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GASP - A COMPUTER CODE FOR CALCULATING THE THERMODYNAMIC AND TRANSPORT PROPERTIES FOR EIGHT FLUIDS - HELIUM, METHANE, NEON, NITROGEN, CARBON MONOXIDE, OXYGEN, ARGON, CARBON DIOXIDE

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SUMMARY

A family of FORTRAN IV subroutines was developed to calculate the thermodynamic and transport properties of eight fluids at pressures from 0.1 to 200 atmospheres (to 100 atm for helium) and from the triple point to 300 K for neon; to 500 K for carbon monoxide and oxygen; to 600 K for methane and nitrogen; to 1000 K for argon and carbon dioxide; and from 3 to 500 K for helium. This paper presents some of the historical basis for the calculations and the equation of state selected. An operations sheet with a detailed description of pertinent input parameters and a discussion of the results is included in the text. A brief description of each subroutine is presented in appendix A. The master subroutine GASP calculates the remaining state variable when given any two of pressure, density, and temperature as input. In addition, any or all of the thermodynamic and transport properties - enthalpy, entropy, specific heats (Cp, Cv), sonic velocity, viscosity, thermal conductivity, surface tension - can be obtained. A call to GASP with pressure and enthalpy or entropy as input will also generate the other properties. A special technique is provided to estimate the thermal conductivity near the thermodynamic critical point.

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The GASP package was developed to be used with heat transfer and fluid flow calculations. Because of this intent, the package was written as a family of independent subroutines with a separate subroutine for each specific property or set of related properties. Thus a user with limited needs can work with only those subroutines required for his program.

Cryogenic fluids are used for cooling equipment, preservation, and destruction of biological specimens, heating or cooling other fluids, as modeling fluids, and in many cases as the primary test fluids in heat transfer and fluid dynamics research. Carbon dioxide is used in many experiments because of its "room temperature" critical temperature.

Cryogenic fluids are used in biology and medicine for the preservation and destruction of tissue. Skin cancers and growths have been successfully treated by spraying liquid nitrogen on the defective tissue (1). Thousands have been treated since 1962 for involuntary movement disorders (parkinsonism, dystonia musculorum deformaus, intention tumor, and tortiocollis), using stereotoxic cryothalamectomy (2). Gynecological disorders have been treated using cryogenic cannula techniques with a variety of freezing surface configurations (3).

A variety of techniques using cryogens are available for the preservation of whole blood and its constituents for periods of years (4). Cryogens have been used to preserve foodstuffs, such as fish, poultry, red meats, fruits and vegetables (mushrooms, tomato slices, peas, beans, berries, sliced peaches, etc.) (5 and 6).

Currently much effort is being devoted to whole organ preservation. The recent work of Lehr (7) indicates that the kidney may be able to survive freezing when microwave energy is used to revitalize the organ. In cryoimmunology, destructive freezing has been shown to stimulate the production of antibodies (8).

Cryogenic fluids are used in the freeze drying of foods, microorganisms, pharmaceuticals, and biologicals (9). Hydrogen and helium bubble chambers are used in nuclear physics (ref. 10). Ultrahigh vacuums can be achieved through cryopumping (ref. 11). Liquid oxygen (LOX) is used at hospitals; in increasing the capacity of sewage plants, and in 1968, 70% of all LOX produced was consumed by the steel industry (ref. 12). High speed trains are proposed which require cryogenically cooled superconducting magnets (ref. 13). Superconducting power transmission equipment will require cryogens, helium (perhaps hydrogen), as well as cryogenic conditioning equipment. Ejectors operating in the cryogenic regime can substantially augment the capacity of refrigeration systems (ref. 14). Cryogens are used to produce a low background noise environment for infrared detection equipment (ref. 15). Cryoelectronics, superconducting motor-generators, and thermonuclear power are all dependent on cryogens.

The problems associated with the liquefaction, storage, and gasification of LNG (liquid natural gas) and LPG (liquid petroleum gas) are currently being studied (ref. 16).

Cryogens are used in metal forming cryoquenching, and for producing higher quality machine tools (refs. 17, 18).

This list of applications is by no means complete and review of other cryogenic applications and several cited herein can be found in references 19, 20, and 21. The point is simply that each of these applications requires not only a knowledge of the thermodynamic and transport properties of the fluid but an efficient readily accessible technique for evaluating these properties.

GASP is a FORTRAN IV family of subroutines which was developed on a 7094-7044 DCS machine (it is also available for the 360 system) to determine the thermodynamic and transport properties of eight fluids (helium, methane, neon, nitrogen, carbon monoxide, oxygen, argon, carbon dioxide) and be used in conjunction with other research programs. The GASP property package is subdivided into subroutines and functions for computing the individual properties. The individual subroutines may be used independently of subroutine GASP if the user's requirements are of a more restricted nature (i.e., memory or time limited). Appendix A is a descriptive breakdown of all the functions and subroutines used by the master subroutine GASP, which is listed in appendix B.

The basis for the program is the work of Bender (ref. 22) and Strobridge (ref. 23). Strobridge curve fit the available nitrogen data with a modified Benedict-Webb-Rubin (BWR) (ref. 24) equation of state.

This work represented a major advance in establishing an equation of state for cryogens. The excellent hydrogen data of Roder and Goodwin (ref. 25) were fit using a form similar to that of reference 23. In the early days of work with cryogenic hydrogen such an equation represented a milestone to those working in research and development.

Bender (ref. 22) added a new constraint to the problem of curve-fitting PVT data and required subcritical data to satisfy the Maxwell-Phase Rule. The use of this constraint, although not well defined in reference 22, can give saturation properties directly from the equation of state. Bender (ref. 22) fit selected PVT data, subject to the Maxwell-Phase Rule constraint, for five fluids: methane, nitrogen, oxygen, argon, and carbon dioxide from the triple point temperature at 1/2 atm to approximately 600 K and 200 atm to within the accuracy of the experimental data. The form of Bender's equation (ref. 22) is based on that of Strobridge (ref. 23). Because the rules for obtaining saturation properties were not clear from reference 23, the saturation properties of these five fluids were calculated herein from curve fits.

Hust and Stewart (ref. 26) used the principle of corresponding states and the equation of Strobridge (ref. 23) to give thermodynamic property values of carbon monoxide. McCarty and Stewart (ref. 27) used a modified form of the Strobridge equation and corresponding states to fit the PVT data for neon. The neon data were subject to the usual critical constraints and one additional constraint; namely that the equation must fit the data for the Joule-Thompson inversion locus.

Mann (ref. 28) further modified Strobridge's equation to fit the available helium data, much of which was compiled by Mann and Stewart (ref. 29). Since that time, R. D. McCarty (ref. 30) has obtained a more exacting fit to the data; furthermore McCarty's fit yields good values of $\partial^2 P/\partial T^2$ for the fluid helium. This is not the case for the equations of Strobridge (ref. 23), Mann (ref. 28), Hust and Stewart (ref. 26), and McCarty and Stewart (ref. 27). Bender's equation (ref. 22) also gives good values of $\partial^2 P/\partial T^2$ for the five fluids fit therein.

The equation of state used in this report is a modification of Bender's original equation (ref. 22) to include the modifications to the Strobridge equation (ref. 23) for the fluids, helium, neon, and carbon monoxide. The primary references used in GASP for thermodynamic and transport property calculations are presented in table I. The equation of state is presented in appendix A, under SUBROUTINE PRESS, and the coefficient matrix for all fluids is presented as table II.

The Bender equation of state (ref. 22) has been compared to the P-ρ-T data of several investigators. Comparisons to data were made for methane, carbon-dioxide, oxygen, argon, and indirectly for nitrogen and helium. In figures 1 through 12, the relative errors in the calculated P, ρ, or T are illustrated as functions of the reduced property for methane and oxygen. For example in figure 2, the relative errors in

pressure $(P_{exp} - P_{calc})/P_{exp}$ are plotted as functions of the reduced pressure P_{exp}/P_{crit}.

The essence of these figures and other comparisons can be partially summarized in table III. However, one should consult the figures in order to more fully understand the deviations between the state equation and the data.

The results were generally in good agreement with the collection of data in Dinn (ref. 32). The fit of the helium data given by McCarty (ref. 30) indicates the helium results to be off as much as 4% in PVT and up to 20% in some derived properties in the near critical region, indicating the helium fit, used herein, will need further modifications. Even the neon densities are not in complete accord with reference 27, and the derived values deviate somewhat from those of reference 27, indicating that these data will also need further modifications.

The GASP property package differs from the various techniques of references 22 through 30 in that it was developed to be used in fluid flow and heat transfer calculations. As such, there are independent calls for the three state variables pressure, density, or temperature (see table IV OPERATIONS SHEET). In addition, temperature and all the other properties can be obtained as a function of pressure and enthalpy, or pressure and entropy which are often used in forced convection studies. Selected examples of properties calculated using GASP are given as figures 14 and 15.

While enthalpy and entropy are available in references 23 to 28 the specific heats (Cp, Cv), sonic velocity, viscosity, thermal conductivity, and surface tension were not computed (good values of Cp and Cv are given for helium in ref. 30). One of the major reasons that the specific heats were not given is the significant deviations in $\partial^2 P/\partial T^2$ at near critical temperatures which generally lead to very large values of Cv. For example, using the Strobridge equation, the calculated values of Cv for nitrogen are illustrated in figure 13. After much effort in this area, the authors finally decided to use numerical techniques to determine $\Delta U/\Delta T = Cv$ and $\Delta H/\Delta T = Cp$, for ρ/ρ_c cutoff value that varies with each fluid. See figure 16 and SUBROUTINE CPPRL, appendix A. The viscosity and thermal conductivity computational methods were adapted from references 33 and 34 for the gaseous regime and from references 35, 36, 37, and 38 for the near-critical regime. The surface tension calculation was adapted from reference 39, and modified to fit the date given in reference 40. A description of the equations for these transport properties is included in appendix A.

The symbols used herein are given in appendix C.

APPENDIX A

FUNCTIONS AND SUBROUTINES CONTAINED IN SUBROUTINE GASP

If the user wishes to disassemble GASP into its family of subroutines, the user should contact the authors at Lewis Research Center, Cleveland, Ohio 44135.

In all cases, the units are specified by KU and the region by KR, see sketch, table IV. If KR is either specified as 1 or returned as 1 the saturated liquid and vapor properties are computed. All saturated properties become available through the labeled common statement COMMON/PROPTY/etc. Three of five choices of KU available to the user are given in table V.

The property routine GASP will warn the user if the input or calculated values are out of range, if an iteration has not converged, or a value has been extrapolated; however, calculation will continue. Calculations will be terminated if the user fails to specify the name of the fluid, see SETUP (NAMGAS).

A flowchart of subroutine GASP and the routines called directly by GASP is included in appendix D.

BLOCK DATA - A Data Subroutine

This routine contains the message which lists the fluid used and the associated critical constants, e.g.,

THERMODYNAMIC AND TRANSPORT PROPERTIES FOR CO2:

PC = 72.869 ATM, TC = 304.21 K, ROC = .464 GM/CC

Also included are the units conversion factors to convert the user's units as specified by KU to those which are internally consistent. KU = 1 gives units which are the same as in the program.

SUBROUTINE SETUP (NAMGAS)

This routine uses NAMGAS, a 2 or 3 letter Hollerith code tabulated below, to select the coefficients for a particular fluid and overlay them into the common blocks needed by GASP. The coefficients include:

(1) Equation of state coefficients

(2) Saturated vapor law coefficients

(3) Specific heat at zero pressure coefficients

(4) Transport coefficients

(a) Viscosity $\mu - \mu^*, \mu^*$

(b) Thermal conductivity $\lambda - \lambda^*, \lambda^*$

(c) Force constants

(d) Surface tension σ

(5) Region delimiters on P, T, ρ, H

(6) Region delimiters for switching to numerical Cv calculation

Fluid	Hollerith code	Fluid	Hollerith code
Helium	HE	Nitrogen	N2
Methane	CH4	Oxygen	02
Neon	NE	Argon	AR
Carbon-monoxide	CO	Carbon-dioxide	CO2

The coefficients for items 1 to 3 and 5 are listed in table II. The references for the other coefficients are listed in the fluid reference table I.

SUBROUTINE CHECKS (A multiple entry subroutine)

ENTRY DCHECK(KU,D)

At this entry point the density D is converted to grams/cm^3 and checked to see if D is out of range.

ENTRY PCHECK(KU,KR,P)

This entry converts the pressure P to mega-Newtons/$(meter)^2$ and checks for out of range. If KR=1, P is checked for out of saturation range. If P is out of range, the program writes an out of range note and continues.

ENTRY TCHECK(KU,KR,T)

This entry converts the temperature T to degrees Kelvin and checks for out of range. If KR=1, T is checked for out of saturation range. If T is out of range, the program writes a note and continues.

This routine is used frequently to insure that the proper regions and units are used in the calculations. It prints OUT OF RANGE messages to

warn the user that the results are extrapolated, and may be incorrect. It is the responsibility of the user to check these results for validity.

FUNCTION SOLVE(X1,F,DF)

This routine is a Newton-Raphson iteration given an initial estimate X1, the function F, and its derivative DF. If the convergence has not been attained in 100 iterations, the result and a note are written out. Calculation continues with the last value.

SUBROUTINE ROOT(XO,X2,FOFX,FUNC,X1)

This routine solves for X1 such that FUNC(X1)=FOFX, where X1 lies between XO and X2. It includes a modified half-interval search technique and permits only one root between XO and X2. If a root has not been found in 100 iterations, the result and a note are written out, and calculation continues.

SUBROUTINE ROOTX - Same as SUBROUTINE ROOT

This routine must be included to allow a function argument of ROOTX to call ROOT.

SUBROUTINE SPLINA(X,Y,NX,T,NT,YINT,KFD,KERROR)

This is a spline curve fit routine used for interpolation.

SUBROUTINE POLY(X,COEF)

This routine evaluates the polynomial at X, where f(x) is described by the coefficient array COEF.

SUBROUTINE DENS(KU,T,P,D,DL,DV,KR)

This routine computes the density D, given the temperature T and pressure P. If KR=1, the saturated liquid and vapor densities, DL and DV, respectively, are computed as a function of T only. If either T or P is initialized to zero, the saturated densities are computed as functions of P or T, respectively, and the saturation temperature or pressure is returned in the initialized store.

SUBROUTINE PRESS(KU,T,D,P,KR)

This routine computes the pressure P, given temperature T and density D. If KR=1, P will be the saturation pressure computed as a function of T only by SUBROUTINE PSSS. While the equation of state is found in SUBROUTINE PRESS, it is also used in subsequent routines. The state equation used by GASP is:

$$P = R\rho T + A(T)\rho^2 + B(T)\rho^3 + C(T)\rho^4 + D(T)\rho^5 + n_{13}\rho^6 + \rho^3[E(T) + \rho^2 F(T)]e^{-n_{20}\rho^2/T_2}$$

where if the fluid is helium, $T_2 = T$, otherwise $T_2 = 1$.

$$A(T) = n_1 T + n_2 + \frac{n_3}{T} + \frac{n_4}{T^2} + \frac{n_5}{T^3} + \frac{n_{21}}{T^4}$$

$$B(T) = n_{22}T^2 + n_6 T + n_7 + \frac{n_8}{T} + \frac{n_{23}}{T^2}$$

$$C(T) = n_9 T + n_{10}$$

$$D(T) = n_{11}T + n_{12} + \frac{n_{24}}{T}$$

$$E(T) = \left(n_{14} + \frac{n_{15}}{T} + \frac{n_{16}}{T^2}\right)\frac{1}{T^2}$$

$$F(T) = \left(n_{17} + \frac{n_{18}}{T} + \frac{n_{19}}{T^2}\right)\frac{1}{T^2}$$

The coefficients n_1 to n_{20} are from Bender's original equation while n_{21} to n_{24} have been added for carbon-monoxide, neon, and helium.

SUBROUTINE TEMP(KU,P,D,T,KR)

This routine computes the temperature T, given pressure P and density D. If KR=1, T will be the saturation value computed as a function of P only, by function TSS.

FUNCTION DSF(DS) (A multiple entry routine)

This is a function used with DENS to solve for density DS given temperature TS and pressure PS.

DSF = P equation of state - P given

ENTRY DDSF(DS)

This routine calculates the derivative of the above function and is used with DENS to solve for density DS given temperature TS and pressure PS

$$DDSF = \frac{\partial(DSF)}{\partial \rho}$$

SUBROUTINE PSSS(PSS)

This routine computes the saturation pressure PSS given temperature TS, where

$$\log_{10} P = j_1 + \frac{j_2}{T} + j_3 T + j_4 T^2 + J_5 T^3 + j_6 T^4 + j_7 T^5$$

and the values j_1 to j_7 are found in SETUP.

FUNCTION TSS(PS)

This is a function used to compute saturation temperature given the pressure PS.

FUNCTION TSSF(TSS) (A multiple entry routine)

This function is used with FUNCTION TSS to solve for saturation temperature TSS given pressure PS.

TSSF = Vapor pressure equation - $\log_{10}$(PS)

ENTRY DTSSF(TSS)

This routine provides the derivative of the above function and is used with function TSS to solve for saturation temperature TSS given the pressure PS

$$DTSSF = \frac{\partial(TSSF)}{\partial T}$$

FUNCTION TSF(TS) (A multiple entry routine)

This function is used with TEMP to solve for the temperature TS, given pressure PS and density DS.

TSF = Equation of state - PS

ENTRY DTSF(TS)

This routine calculates the derivative of the above function and is used with TEMP to solve for temperature TS given pressure PS and density DS.

$$DTSF = \frac{\partial(TSF)}{\partial T}$$

SUBROUTINE TEMPPH(KU,P,H,T,D,DL,DV,KR)

For a given pressure P and enthalpy H, this routine will return values of temperature T and density D. If KR=1, saturated liquid and vapor properties will be returned.

SUBROUTINE TEMPPS(KU,P,S,T,D,DL,DV,KR)

For a given pressure P and entropy S, this routine will return values of temperature T, and density D. If KR=1, saturated liquid and vapor properties will be returned.

FUNCTION TSHF(TS) (A multiple entry routine)

This is a function used in conjunction with TEMPPH. It obtains a trial value of DS using the given PS and a trial TS. Then it obtains a trial H which is compared to the input enthalpy within an iteration in TEMPPH.

ENTRY TPSF(TS)

This is a function used in conjunction with TEMPPS. It obtains a trial value of DS from the given PS and a trial TS. Then it finds a trial S which is compared to the input entropy within an iteration in TEMPPS.

SUBROUTINE ENTH(KU,KR,T,P,D,H,HL,HV)

This routine computes enthalpy H given the temperature T, pressure P, and density D. If KR=1, the saturated liquid and vapor enthalpies HL and HV, respectively, are computed as a function of T only.

SUBROUTINE ENT(KU,KR,T,P,D,S,SL,SV)

This routine computes entropy S given temperature T, pressure P, and density D. If KR=1, the saturated liquid and vapor entropies SL and SV, respectively, are computed as a function of T only.

FUNCTION HDINT(DS,DSL) (A multiple entry routine)

This routine computes the integral used in the enthalpy computation from density DSL to density DS.

$$\Delta H = \int_{DSL}^{DS} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_\rho \right]_T d\rho$$

ENTRY SDINT(DS,DSL)

This routine computes the entropy integral from the density DSL to the density DS

$$\Delta S = \int_{DSL}^{DS} \left[-\frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_\rho \right]_T d\rho$$

FUNCTION HDINTF(DS) (A multiple entry routine)

This routine evaluates the integrand of function HDINT where DS is the variable of integration.

$$\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_\rho$$

ENTRY SDINTF(DS)

This routine evaluates the integrand of function SDINT where DS is the variable of integration.

$$-\frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_\rho$$

FUNCTION HSS(PS,DS) (A multiple entry routine)

This function computes the enthalpy in the region KR=3 (see table IV) or saturated vapor enthalpy (KR=1), given pressure PS, density DS, and temperature TS.

$$H = H^0 + \int_{T_0}^{T} Cp_0 \, dT + (Z - 1)RT + \int_0^{\rho} \left[\frac{P}{\rho^2} - \frac{T}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_\rho \right]_T d\rho$$

where

$$Cp_0 = \sum_{i=1}^{5} m_i T^{i-1}$$

and the values m_1 to m_5 are found in SETUP.

ENTRY SSS(PS,DS)

This routine computes the entropy in region KR=3 or the saturated vapor entropy (KR=1) given the pressure PS, the density DS, and temperature TS.

$$S = S^0 + \int_{T_0}^{T} Cp_0 \, d(\ln T) - R \ln(RT\rho) + \int_0^{\rho} \left[\frac{R}{\rho} - \frac{1}{\rho^2} \left(\frac{\partial P}{\partial T} \right)_T \right] d\rho$$

SUBROUTINE HSLV(PS) (A multiple entry routine)

This routine is used in conjunction with HSS to compute the saturated liquid and vapor enthalpies given pressure PS and temperature TS. HV comes from HSS, and

HL = HV - T*HSSLVF

ENTRY SSLV(PS)

This routine is used with SSS to compute the saturated liquid and vapor entropies given pressure PS and temperature TS. SV comes from SSS, and

SL = SV - HSSLVF

FUNCTION HSSLVF(PS)

This is a function used with HSLV to compute saturated liquid enthalpy from saturated vapor enthalpy or saturated liquid entropy from saturated vapor entropy given pressure PS and temperature TS.

$$HSSLVF = \frac{\partial P}{\partial T} \Delta V$$

where

$$V = \frac{1}{\rho}$$

SUBROUTINE CPPRL (PS,DS,T,CPPART,CVPART,KU,KR,KCP)

This routine computes the specific heats at constant volume (CV) and constant pressure (CP). IF KR=1, the saturated liquid and vapor specific heats at constant volume, CVL or CVV, and constant pressure CPL or CPV, respectively, are computed as requested by GASP.

The specific heats are computed by

$$CV = Cp_0 - R - \int_0^{\rho} \frac{T}{\rho^2} \left(\frac{\partial^2 P}{\partial T^2} \right)_{\rho} d\rho$$

$$Cp = CV + \frac{T}{\rho^2} \frac{(\partial P/\partial T)_\rho^2}{(\partial P/\partial \rho)_T}$$

provided the input density is less than ρ_{switch} (ρ_c = critical density). Also see figure 36.

Fluid	ρ_{switch}/ρ_c
Helium	2.4
Methane	2.5
Neon	1.0
Nitrogen	2.2
Carbon monoxide	2.4
Oxygen	2.4
Argon	2.4
Carbon dioxide	2.4

If density is greater than these values, the specific heats are calculated using SUBROUTINE SPCHV.

In addition, if $T < T_{critical}$, then the specific heats for neon, carbon-monoxide, and helium will be computed by SPCHV.

The partial derivatives $(\partial P/\partial T)\rho$ and $(\partial P/\partial \rho)T$ are available to the user in COMMON/PARTLS/PTV,PDT.

FUNCTION CPPRLF(DS)

This routine evaluates the integral used in computing specific heats.

$$CPPRLF = \int \frac{T}{\rho^2} \left(\frac{\partial^2 P}{\partial T^2}\right)_\rho d\rho$$

SUBROUTINE PTRHO(D,T)

This routine evaluates two partial derivatives. The answers are returned in COMMON/PARTLS/PTV,PDT.

$$PTV = \left(\frac{\partial P}{\partial T}\right)_\rho$$

$$PDT = \left(\frac{\partial P}{\partial \rho}\right)_T$$

SUBROUTINE SPCHV(KU,KR,T,P,D,CV,CVL,CVV)

This routine computes the specific heat at constant volume CV given temperature T, pressure P, and density D. If KR=1, the saturated liquid or vapor specific heat, CVL or CVV, respectively, is computed as requested by GASP.

$$CV = \frac{\Delta U}{\Delta T} = \frac{\Delta\left(H - \frac{P}{\rho}\right)}{\Delta T}$$

See SUBROUTINE CPPRL.

SUBROUTINE CVPS(KVP,KR,CVS)

Given temperature, pressure, and density, this routine is used to determine five values of internal energy U for a spline fit used in SPCHV to compute the specific heat at constant volume.

SUBROUTINE SONIC(KU,KR,T,D,GAMMA,C)

This routine computes sonic velocity C given temperature T, density D, and the specific heat ratio GAMMA=CP/CV.

SUBROUTINE VISC(KU,KR,T,D,MU)

This routine computes the viscosity MU, given temperature T and density D. The dilute gas viscosity is computed as a simplified form of the Chapman-Enskog model by $\mu^* = 0.2669\ E - 4\sqrt{mT}/\sigma\alpha^2\Omega_\mu$, where Ω_μ is the Leonard-Jones potential viscosity collision integral, reference 16. The excess viscosity correlation is from Josci, Stiel, and Thodos, reference 13.

$$[(\mu - \mu^*)\xi\times 10^{-4}]^{1/4} = 0.1023 + 0.023364\ \rho_R + 0.058533\ \rho_R^2 - 0.040758\ \rho_R^3 + 0.0093324\ \rho_R^4$$

where $\mu - \mu^*$ data has been verified in the references listed in table I. Here $\rho_R = \rho/\rho_c$ and $\xi = T_c^{1/6}/m^{1/2}P_c^{2/3}$

SUBROUTINE THERM(KU,KR,T,P,D,EXCESK,FK)

This routine computes the thermal conductivity FK, given the temperature T and density D. FK represents the thermal conductivity of the dilute gas plus the excess conductivity ($\lambda - \lambda^*$) which is a function of density. The computation of the thermal conductivity anomaly EXCESK (λ_R) is based on the theory of Sengers and Keys, reference 43, which agrees with the reacting gas theory of Brokaw, reference 41. The techniques are compared and discussed in reference 44.

EXCESK will be computed for the density regime $0.3 < \rho/\rho_c < 1.8$. To obtain the thermal conductivity of a near-critical fluid, the user must add FK and EXCESK.

The dilute gas conductivity and the excess conductivity are curve fits from the data in the references as listed in the fluid reference table I. The Stiel and Thodos correlation of reference 36 is used where it is practical. Special procedures are followed for helium as indicated in the references of table I.

SUBROUTINE SURF(KU,KR,T,SIGMA)

Compute the surface tension SIGMA, given the temperature T, by a corresponding-state correlation suggested by Brock and Bird, reference 39.

SUBROUTINE DGUES(TS,TCR,DST)

This routine provides a near critical density estimate used by subroutine DENS.

FUNCTION CONZ(TEMP)

This routine computes the thermal conductivity of helium for the dilute gas as a function of temperature by the technique of Roder, reference 55.

In closing, now that the reader is familiar with GASP, turn to page 31, excise tables IV and V and discard the remainder of the paper.

APPENDIX B

A LIST OF SUBROUTINE GASP

```
$IBFTC GASPY   DECK
C
C     ------------------NASA  LEWIS  RESEARCH-----------------------------------
C     ------------------------------VERSION 4/19/71
C     -----------FOR  INFORMATION --SEE  A.BARON, R.C.HENDRICKS, J.PELLER-------
C
      SUBROUTINE GASP(KS,KP,T,P,D,H,KR)
C      BENDER-S EQUATION OF STATE FOR THE FIVE GASES--N2,CH4,AR,O2,CO2
C       ALSO EQUATIONS OF STATE FOR CO, NE, AND HELIUM...
C ------------------------- PRYDZ EQUATION FOR FLUORINE ---------------
C
C        COMPUTE THE STATE RELATIONS AND THERMODYNAMIC AND
C        TRANSPORT PROPERITES OF SPECIFIED FLUID GIVEN TEMPERATURE T,
C        PRESSURE P, DENSITY D, OR ENTHALPY H.  STATE RELATIONS ARE
C        SPECIFIED BY KS.  THERMODYNAMIC AND TRANSPORT PROPERTIES
C        ARE SPECIFIED BY KP.  IF KR IS RETURNED OR SPECIFIED AS 1,
C        PROPERTIES ARE COMPUTED AT SATURATION.
C
      DIMENSION KPC1(32), KPC2(32), KPC3(32),KPC4(32)
      COMMON/PROPTY/KU,DL,DV,HL,HV,S,SL,SV,CV,CVL,CVV,CP,CPL,CPV,GAMMA,
     1GAMMAL,GAMMAV,C,CL,CVP,MU,MUL,MUV,K,KL,KV,SIGMA,EXCL,EXCV,EXCESK
      REAL MU,MUL,MUV,K,KL,KV
      COMMON/CHECKS/DCH1    ,DCH2,PCH1,PCH2,PCH3,TCH1,TCH2,TCH3,DST,TST,H
     1SCH1,HSCH2
      DATA KPC1 /2,3,6,7,10,11,14,15,18,19,22,23,26,27,30,31,34,35,38,
     139,42,43,46,47,50,51,54,55,58,59,62,63/
      DATA KPC2 /4,5,6,7,12,13,14,15,20,21,22,23,28,29,30,31,36,37,38,
     139,44,45,46,47,52,53,54,55,60,61,62,63/
      DATA KPC3 /8,9,10,11,12,13,14,15,24,25,26,27,28,29,30,31,40,41,42,
     143,44,45,46,55,56,57,58,59,60,61,62,63/
      DATA KPC4 /16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,
     148,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63/
      GO TO (10,20,30,40,45),KS
C
C        COMPUTE DENSITY
C
   10 IF (KR.NE.1.AND.(P.LT.PCH1.OR.T.LT.TCH1))WRITE(6,251)
      IF (KR.EQ.1.AND.(P.LT.PCH1.AND.T.LT.TCH1)) WRITE(6,252)
      IF (P.GT.PCH3.OR.T.GT.TCH3) WRITE(6,253)
      CALL DENS(KU,T,P,D,DL,DV,KR)
      GO TO 50
C
C        COMPUTE PRESSURE
C
   20 IF (KR.NE.1.AND.(T.LT.TCH1.OR.D.LT.DCH1) ) WRITE(6,251)
      IF (KR.EQ.1.AND.(T.LT.TCH1.AND.D.LT.DCH1)) WRITE(6,252)
      IF (T.GT.TCH3.OR.D.GT.DCH2) WRITE(6,253)
      CALL PRESS(KU,T,D,P,KR)
      GO TO 50
C
C        COMPUTE TEMPERATURE
C
   30 IF (KR.EQ.1.AND.(P.LT.PCH1.AND.D.LT.DCH1)) WRITE(6,251)
      IF (KR.NE.1.AND.(P.LT.PCH1.OR.D.LT.DCH1)) WRITE(6,252)
      IF (P.GT.PCH3.OR.D.GT.DCH2) WRITE(6,253)
      CALL TEMP(KU,P,D,T,KR)
      GO TO 50
C
C        COMPUTE TEMPERATURE AND DENSITY GIVEN PRESSURE AND ENTHALPY
C
   40 IF (P.LT.PCH1.OR.P.GT.PCH3) WRITE(6,254)
      CALL TEMPPH(KU,P,H,T,D,DL,DV,KR)
      GO TO 50
C
C        COMPUTE  TEMPERATURE  AND  DENSITY  GIVEN  PRESSURE  AND  ENTROPY
C
   45 IF ( P .LT. PCH1 .OR. P .GT. PCH3 ) WRITE (6,254 )
      CALL TEMPPS ( KU,P,S,T,D,DL,DV,KR )
   50 IF (MOD(KP,2)) 60,70,60
```

```
C
C        COMPUTE ENTHALPY
C
   60 CALL ENTH(KU,KR,T,P,D,H,HL,HV)
   70 DO 80 I=1,32
      IF (KP-KPC1(I))110,100,80
   80 CONTINUE
      GO TO 110
C
C        COMPUTE ENTROPY
C
  100 CALL ENT(KU,KR,T,P,D,S,SL,SV)
  110 DO 120 I=1,32
      IF(KP-KPC2(I)) 140,130,120
  120 CONTINUE
      GO TO 140
  130 KCP=0
C
C        COMPUTE  SPECIFIC  HEATS  AND  SONIC  VELOCITY
C
      IF (KR.NE.1) GO TO 200
      CALL DENS(KU,T,P,D,DL,DV,1)
      CALL CPPRL(P,DL,T,CPL,CVL,KU,KR,KCP)
      CALL CPPRL(P,DV,T,CPV,CVV,KU,KR,KCP)
      GAMMAL=CPL/CVL
      GAMMAV=CPV/CVV
      CALL SONIC(KU,KR,T,DL,GAMMAL,CL)
      CALL SONIC(KU,KR,T,DV,GAMMAV,CVP)
      GO TO 140
  200 CALL CPPRL(P,D,T,CP,CV,KU,KR,KCP)
      GAMMA=CP/CV
      CALL SONIC(KU,KR,T,D,GAMMA,C)
  140 DO 150 I=1,32
      IF (KP-KPC3(I)) 170,160,150
  150 CONTINUE
      GO TO 170
C
C        COMPUTE VISCOSITY
C
  160 IF (KR.NE.1) GO TO 165
      CALL DENS(KU,T,P,D,DL,DV,1)
      CALL VISC(KU,KR,T,DL,MUL)
      CALL VISC(KU,KR,T,DV,MUV)
      GO TO 170
  165 CALL VISC(KU,KR,T,D,MU)
  170 DO 175 I=1,32
      IF(KP-KPC4(I)) 190,180,175
  175 CONTINUE
      GO TO 190
C
C        COMPUTE THERMAL CONDUCTIVITY
C        NOTE-- FROZEN  VALUE  AVAILABLE  IN K,KL,KV
C           --  REACTING  CONDUCTIVITY  RETURNED  IN  EXCESK, EXCL,EXCV
C
  180 IF (KR.NE.1) GO TO 220
      CALL DENS(KU,T,P,D,DL,DV,1)
      CALL THERM (KU,KR,P,T,DL,EXCL,KL)
      CALL THERM (KU,KR,P,T,DV,EXCV,KV)
      GO TO 190
  220 CALL THERM (KU,KR,P,T,D,EXCESK,K)
  190 IF(KP-32) 230,240,240
C
C          COMPUTE SURFACE TENSION
C
  240 CALL SURF (KU,KR,T,SIGMA)
  230 RETURN
  251 FORMAT(1H0,45H OUT OF RANGE-LOW-SEE ERROR LIST-CALC.CONT
  252 FORMAT(1H0,45H OUT OF RANGE-SAT-SEE ERROR LIST-CALC.CONT
  253 FORMAT(1H0,45H OUT OF RANGE-HI -SEE ERROR LIST-CALC.CONT
  254 FORMAT(1H0,45H OUT OF RANGE- P -SEE ERROR LIST-CALC.CONT
      END
```

APPENDIX C

SYMBOL LIST

	Fortran symbol*	
c	C	sonic velocity, cm/sec
	CL	sonic velocity, saturated liquid, cm/sec
	CVP	sonic velocity, saturated gas, cm/sec
Cp	CP	specific heat at constant pressure, J/(g)(K)
Cp_0		specific heat at "zero" pressure, J/(g)(K)
	CPOCOR	specific heat units correction factor
	CPL	saturated liquid specific heat, Cp, J/(g)(K)
	CPV	saturated vapor specific heat, Cp, J/(g)(K)
Cv	CV	specific heat at constant volume, J/(g)(K)
	CVL	saturated liquid specific heat, Cv, J/(g)(K)
	CVV	saturated vapor specific heat, Cv, J/(g)(K)
ρ	D	density, g/cm^3
	DL	density, saturated liquid, g/cm^3
	DS	density used internal to the program, gm/cm^3
	DSL	density, saturated liquid, used internal to the program, gm/cm^3
ρ_t		triple point density, g/cm^3
	DV	density, saturated vapor, g/cm^3
	EXCL	reacting conductivity, saturated liquid, w/cm-k
	EXCV	reacting conductivity, saturated vapor, w/cm-k
λ_R	EXCESK	reacting conductivity, w/cm-K

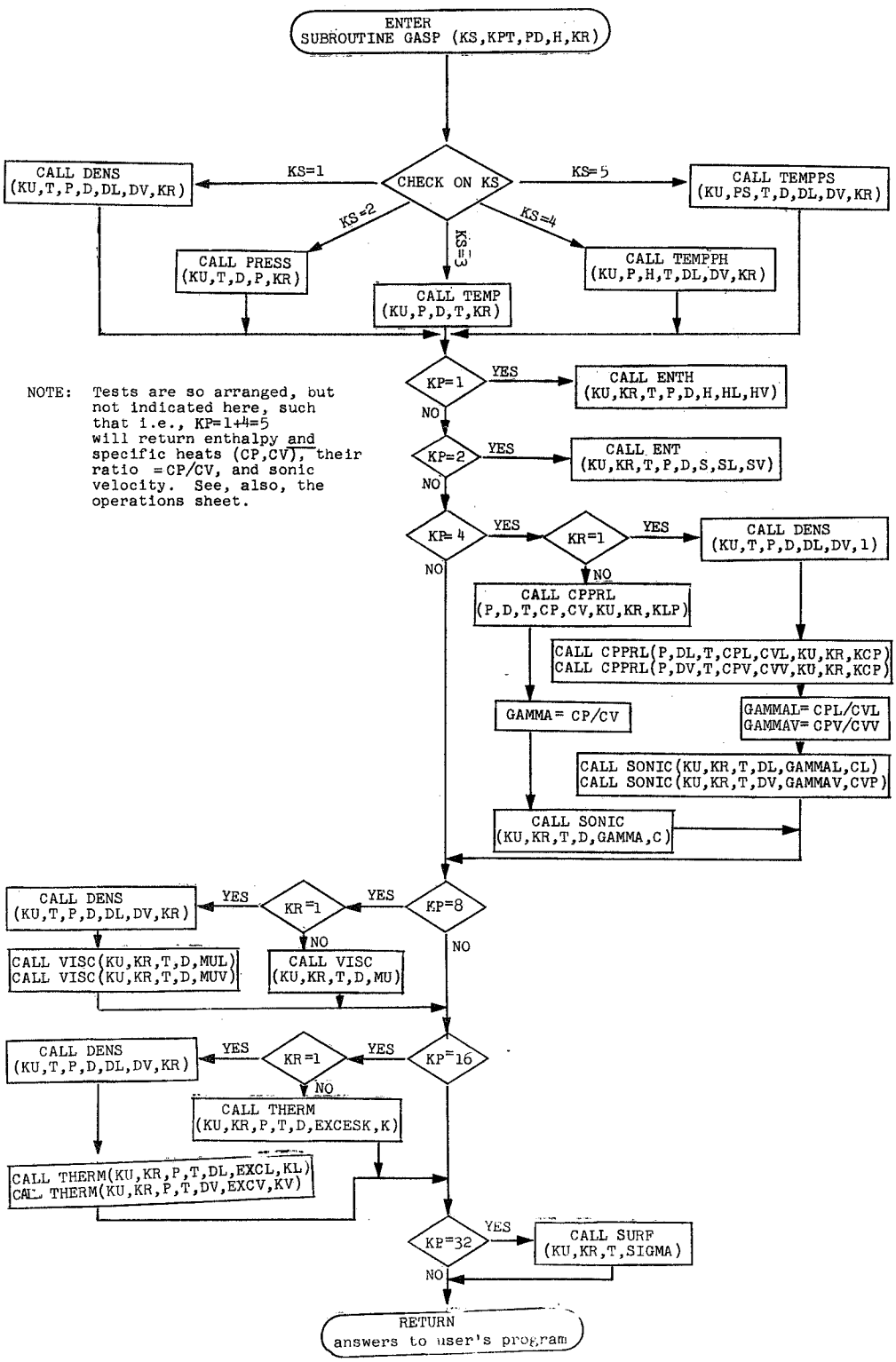
*Symbols used in the individual subroutines are identified in the work statement of that subroutine (see appendix A).

γ	GAMMA	ratio of specific heats, Cp/Cv
	GAMMAL	ratio of specific heats, saturated liquid
	GAMMAV	ratio of specific heats, saturated vapor
H	H	enthalpy, J/g
H_0		reference enthalpy, J/g
	HV	enthalpy, saturated vapor, J/g
	HL	enthalpy, saturated liquid, J/g
j_{1-7}	set	set of constants, equation of vapor pressure curve
k^*		thermal conductivity ($p \rightarrow 0$) W/(cm)(K)
k	K	thermal conductivity, W/(cm)(K)
	KCP	region delimiter used in the numerical calculation of CV
	KL	thermal conductivity, saturated liquid, W/(cm)(K)
	KP	thermodynamic and transport properties specification
	KR	thermodynamic region specification
	KS	state relation specification
	KU	units specification
	KV	thermal conductivity, saturated vapor, W/(cm)(K)
$\mathcal{m}$		molecular weight
m_{1-5}		set of constants, equation of specific heat at "zero" pressure
μ	MU	dynamic viscosity, saturated liquid, g/(cm)(sec)
	MUL	dynamic viscosity, saturated liquid, g/(cm)(sec)
	MUV	dynamic viscosity, saturated vapor, g/(cm)(sec)
n_{1-24}		set of constants, equation of state
P	P	pressure, atm

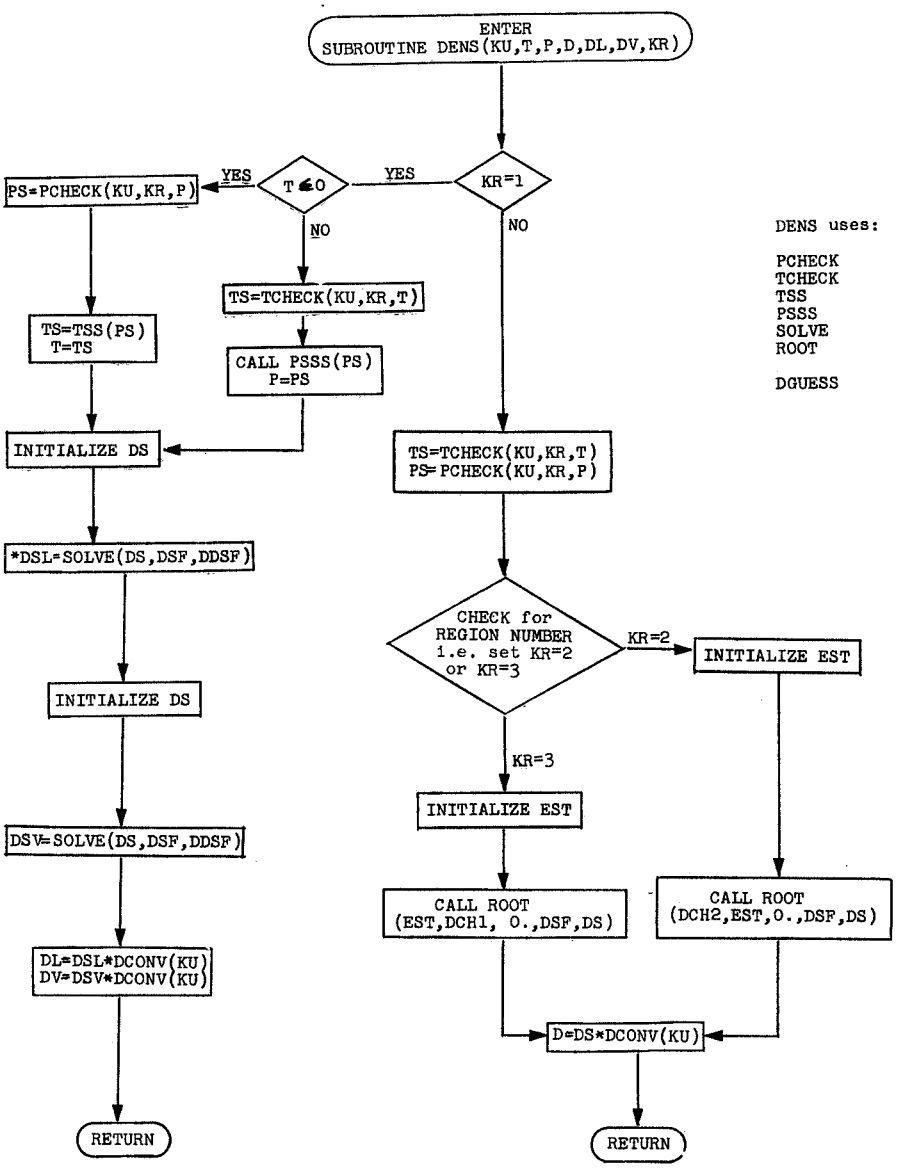
P_c	PC	pressure at the thermodynamic critical point
P_{max}		upper pressure limit, MN/m^2
P_{min}		lower pressure limit, MN/m^2
	PS	pressure used internal to the program, MN/m^2
	PSS	saturation pressure used internal to the program, MN/m^2
	R	gas constant, J/(g)(K)
ρ_c	RHOC	density at the thermodynamic critical point, gm/cm^3
ρ_{switch}		density where calculation of CV change from numeric to analytic
S	S	entropy, J/(g)(K)
σ	SIGMA	surface tension, dyne/cm
σ_d		hard sphere collision diameter, angstroms
S_0		reference entropy, J/(g)(K)
	SL	entropy, saturated liquid, J/(g)(K)
	SV	entropy, saturated vapor, J/(g)(K)
T	T	temperature, K
T_0		reference temperature, K
T_c	TC	temperature of the thermodynamic critical point, K
T_{max}		upper temperature limit, K
	TS	temperature used internal to the program, K
	TSS	saturation temperature computed by FUNCTION TSS, K
T_t		triple point temperature, K
$U = H - \frac{P}{\rho}$		internal energy, J/gm
V		specific volume, cm^3/gm
$Z = \frac{P}{\rho RT}$		compressibility factor
Ω_μ		Leonard-Jones collision integral-viscosity

APPENDIX D

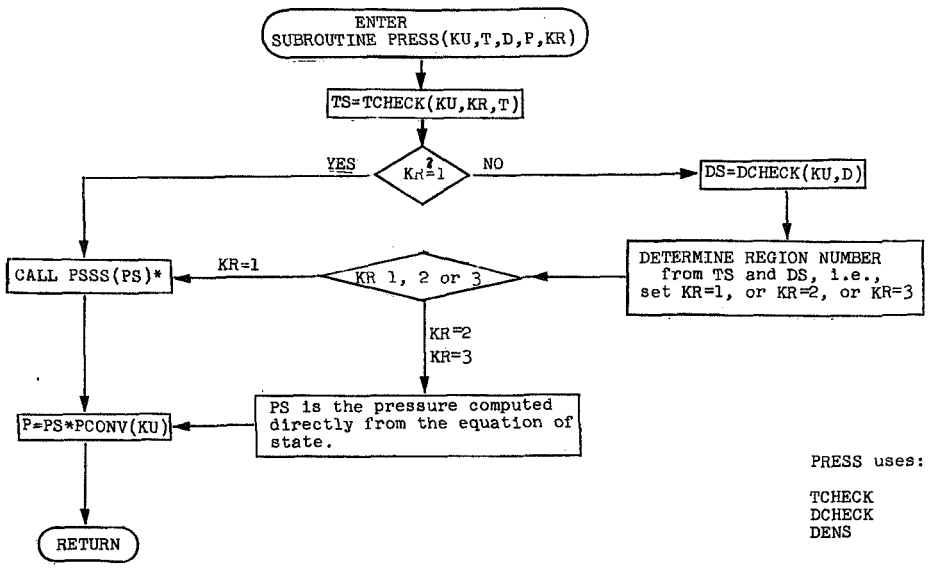
COMPACT FLOW CHART FOR GASP



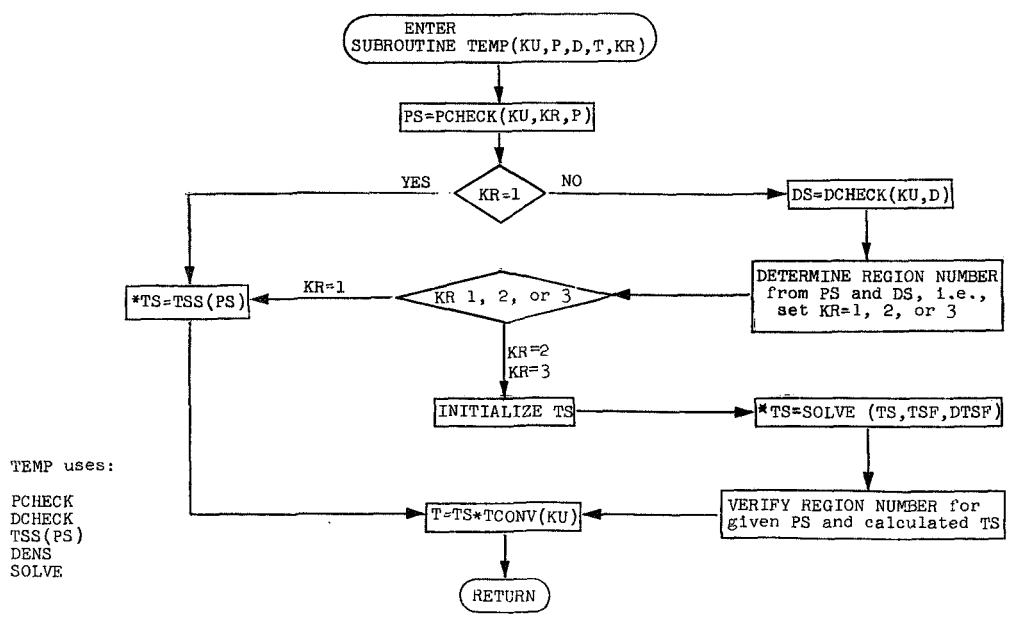
NOTE: Tests are so arranged, but not indicated here, such that i.e., KP=1+4=5 will return enthalpy and specific heats (CP,CV), their ratio =CP/CV, and sonic velocity. See, also, the operations sheet.



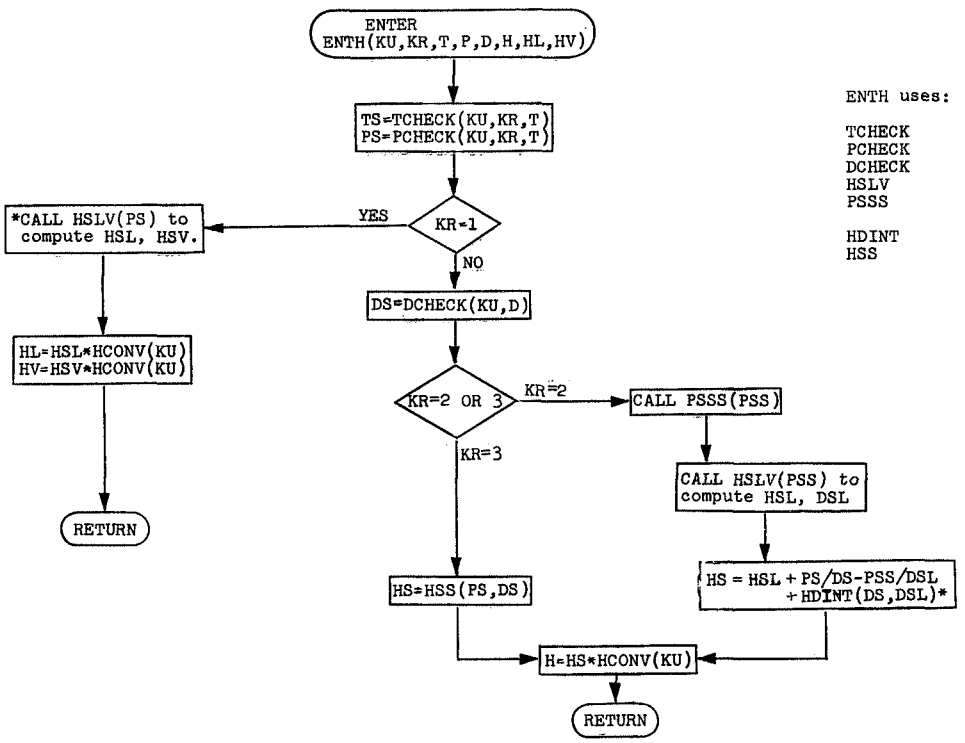
*See APPENDIX A for details of subroutine or function specified.

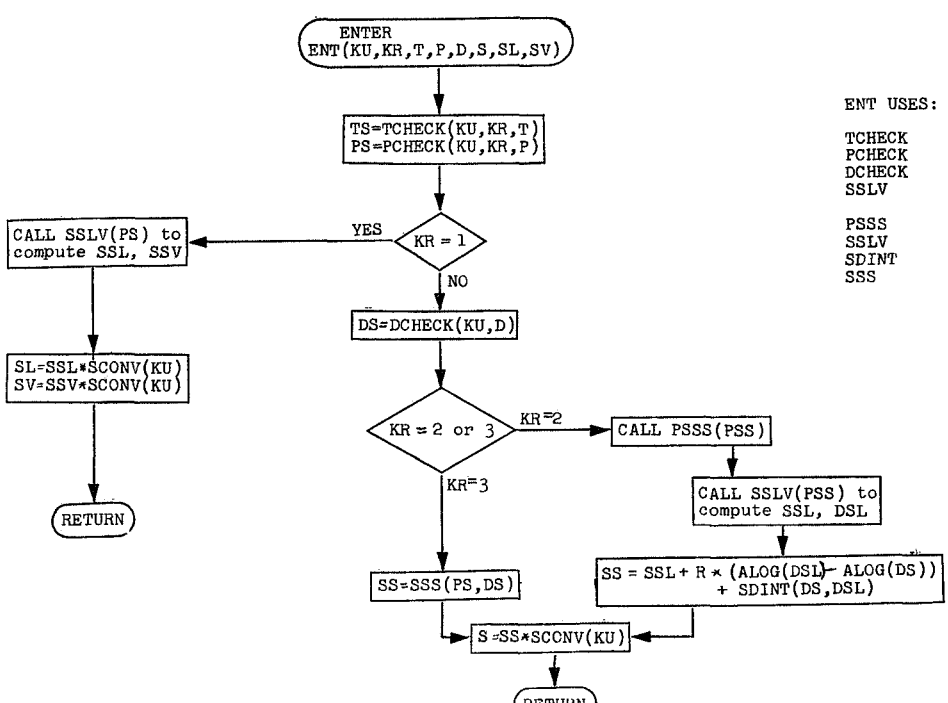


*See APPENDIX A for details of subroutine or function specified.

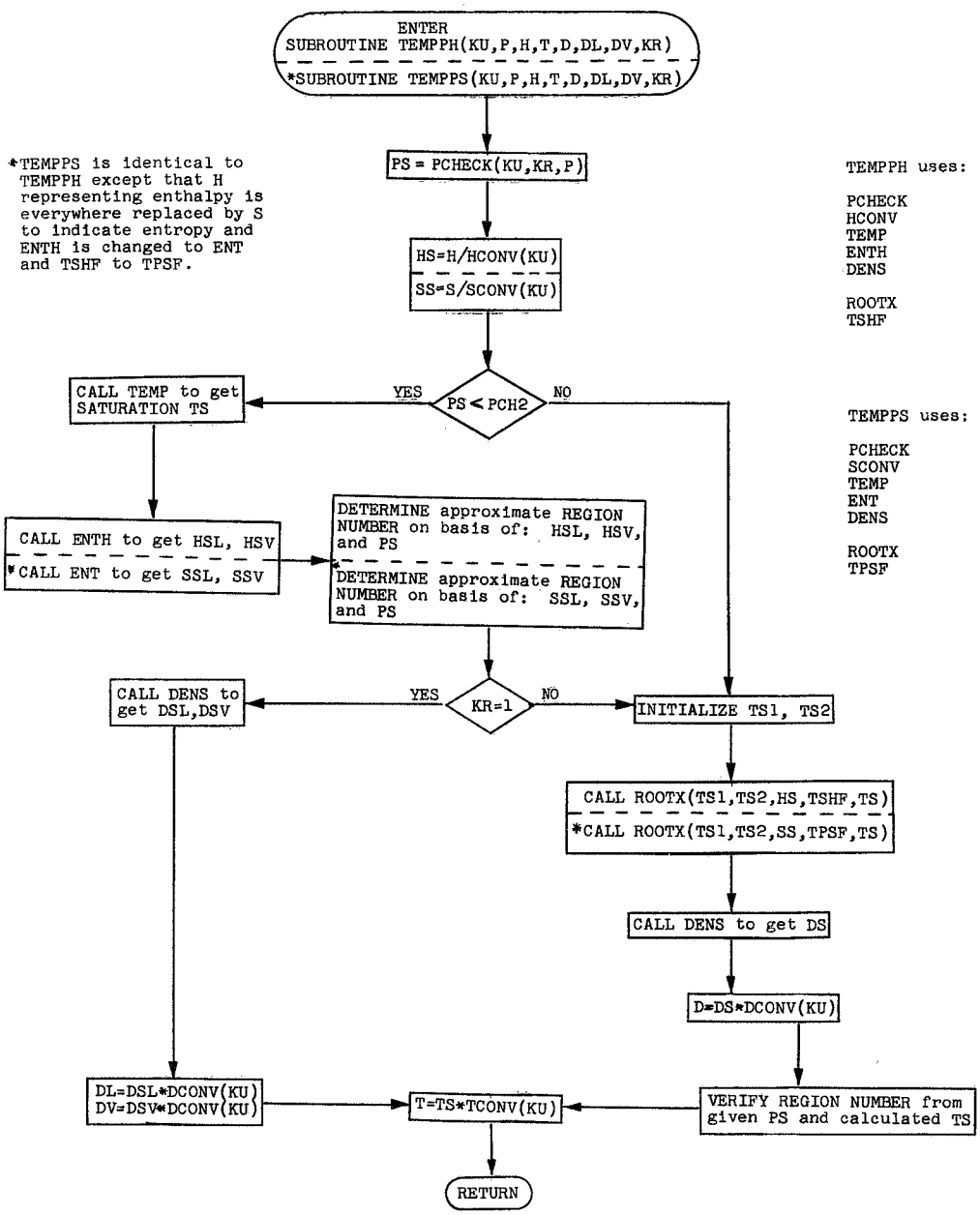


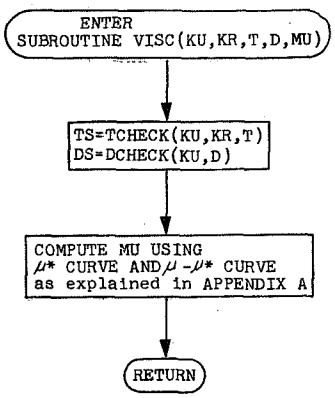
*See APPENDIX A for details of subroutine or function specified.





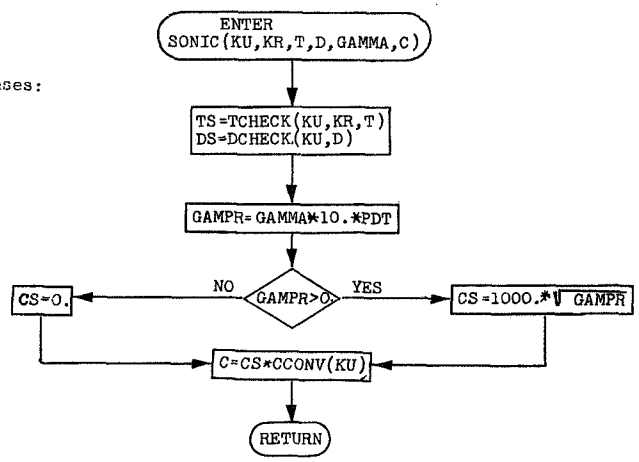
*See APPENDIX A for details of subroutine or function specified.


ENTER
SUBROUTINE TEMPPH(KU,P,H,T,D,DL,DV,KR)
*SUBROUTINE TEMPPS(KU,P,H,T,D,DL,DV,KR)
*TEMPPS is identical to TEMPPH except that H representing enthalpy is everywhere replaced by S to indicate entropy and ENTH is changed to ENT and TSHF to TPSF.
PS = PCHECK(KU,KR,P)
HS=H/HCONV(KU)
SS=S/SCONV(KU)
PS < PCH2
YES
NO
CALL TEMP to get SATURATION TS
CALL ENTH to get HSL, HSV
*CALL ENT to get SSL, SSV
DETERMINE approximate REGION NUMBER on basis of: HSL, HSV, and PS
*DETERMINE approximate REGION NUMBER on basis of: SSL, SSV, and PS
KR=1
CALL DENS to get DSL,DSV
INITIALIZE TS1, TS2
CALL ROOTX(TS1,TS2,HS,TSHF,TS)
*CALL ROOTX(TS1,TS2,SS,TPSF,TS)
CALL DENS to get DS
D=DS*DCONV(KU)
DL=DSL*DCONV(KU)
DV=DSV*DCONV(KU)
T=TS*TCONV(KU)
VERIFY REGION NUMBER from given PS and calculated TS
RETURN
TEMPPH uses:
PCHECK
HCONV
TEMP
ENTH
DENS
ROOTX
TSHF
TEMPPS uses:
PCHECK
SCONV
TEMP
ENT
DENS
ROOTX
TPSF



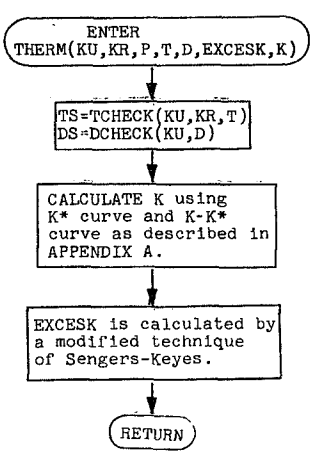
VISC uses:

TCHECK
DCHECK
POLY



SONIC uses:

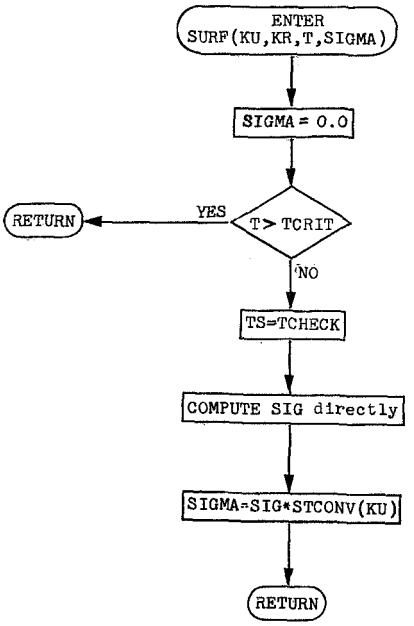
TCHECK
DCHECK



THERM uses:

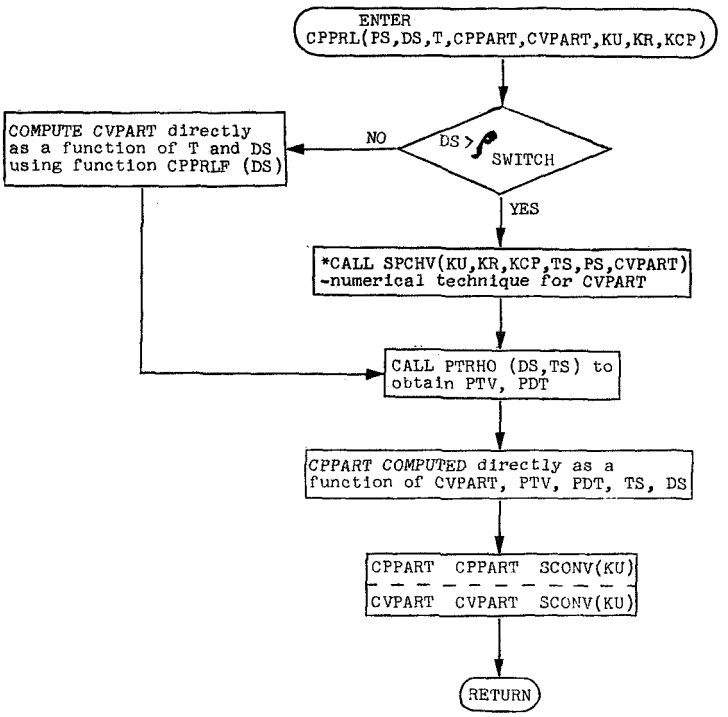
TCHECK
DCHECK
POLY

CONZ



SURF uses:

TCHECK



CPPRL uses:

CPPRLF
SPCHV
PTRHO

TABLE I. - PRIMARY REFERENCES USED IN DERIVED AND TRANSPORT PROPERTY CALCULATIONS

	CH_4	N_2	O_2	Ar	CO_2	Ne	CO	He	F_2
Saturation curve	45	23	31	46	47	48	26	49	See also ref. 56
Cp_0 curve	32	23	33	34	32	34	26	34	57
T_0, S_0, H_0	32	23	31	50	32	37	26	38	
K_0/K^*_{Tc}	51	52	52	53	54	53	52	55	
$K - K^*$	51	52	52	53	54	Using Ar with Ne, Zc, λ 53	Using N_2 with λ, Zc	38	
Surface tension data	40	40	40	40	40	40	40	40	57
K_0 data	34	34	34	34	34	34	34	34	
K data									
μ_0 data	34	34	34	34	34	34	34	34	
μ data									

TABLE II. - COEFFICIENT MATRIX FOR SUBROUTINE SETUP (NAMGAS)

	CH_4	N_2	O_2	Ar	CO_2	Ne	CO	He
EQUATION OF STATE								
R	0.51825100E+00	0.29679700E+00	0.25983199E+00	0.20812800E+00	0.18891799E+00	0.41185435E+00	0.29692807E+00	0.20772224E+01
n_1	0.14305273E+01	0.49288756E+00	0.34811077E+00	0.19825920E+00	0.22488558E+00	0.42879277E+00	0.36547544E+00	0.84477245E+01
n_2	-0.68669271E+03	-0.14910717E+03	-0.14070678E+03	-0.81733119E+02	-0.13717965E+03	-0.41617333E+02	-0.80241533E+02	-0.23475643E+03
n_3	-0.10426391E+05	-0.51324859E+03	0.25061744E+04	0.17777470E+04	-0.14430214E+05	-0.15368388E+04	-0.16713841E+05	0.47857562E+02
n_4	-0.10385156E+08	-0.84144106E+06	-0.10081345E+07	-0.82406544E+06	-0.29630491E+07	0.21705583E+05	0.13129095E+06	-0.11937548E+03
n_5	0.26558245E+09	0.14982437E+08	0.19074164E+08	0.31666098E+08	-0.20606039E+09	0.	0.	0.
n_6	0.38230817E+01	0.50278014E-01	-0.40134966E-02	-0.44202671E-01	0.45554393E-01	0.52377789E-01	0.65308710E+00	0.20230185E+02
n_7	-0.67867615E+03	0.80703712E+02	0.65172112E+02	0.62161423E+02	0.77042840E+02	0.31832376E+02	-0.80131497E+02	0.14653521E+04
n_8	0.28683296E+06	0.99557130E+04	0.10962206E+05	0.11443248E+04	0.40602371E+05	0.15304725E+04	0.	0.
n_9	0.12844809E+02	0.23770201E+01	0.69721580E+00	0.47797520E+00	0.40029509E+00	0.86991276E+00	0.73365157E+00	0.
n_{10}	-0.62715715E+04	-0.59987381E+03	-0.26242449E+03	-0.19645227E+03	-0.39436077E+03	-0.86565802E+02	0.	-0.11186866E+05
n_{11}	0.18343618E+02	-0.86978410E+00	0.19137800E+00	-0.21572754E+00	0.12115286E+00	0.	0.	0.
n_{12}	0.39140891E+04	0.48853747E+03	0.29416771E+02	0.16544141E+03	0.10783386E+03	0.	0.	0.76324486E+05
n_{13}	0.16424545E+05	0.16786859E+03	0.78932076E+02	-0.28142112E+02	0.43962336E+02	0.41994280E+02	0.41363247E+03	-0.70728125E+05
n_{14}	-0.55695049E+08	-0.20154592E+07	-0.19231580E+07	0.82532058E+05	-0.36515545E+08	0.23856729E+06	0.18061147E+07	-0.79046072E+04
n_{15}	0.17955124E+11	0.42241031E+09	0.46108240E+09	-0.91538377E+07	0.19490511E+11	-0.10444366E+08	0.63943277E+09	0.54530768E+05
n_{16}	-0.12157156E+13	-0.20472157E+11	-0.39936263E+11	-0.18340752E+10	-0.29186718E+13	0.	-0.66472139E+11	0.15941147E+06
n_{17}	0.49093507E+09	-0.10052315E+08	-0.56689950E+07	-0.33858136E+07	0.24358627E+08	-0.19828098E+07	-0.24767075E+08	-0.18259780E+07
n_{18}	0.17199887E+12	0.42431222E+10	0.13644286E+10	0.15532886E+10	-0.37546530E+11	0.70965701E+08	0.96546154E+10	0.41462568E+07
n_{19}	0.73467195E+13	-0.39023902E+11	0.91977197E+11	-0.67479568E+11	0.11898141E+14	0.	-0.47286423E+12	-0.16887829E+08
n_{20}	0.37000000E+02	0.10000000E+02	0.54000000E+01	0.35000000E+01	0.50000000E+01	0.13590153E+02	0.74632444E+01	0.40570426E+03
n_{21}	0.	0.	0.	0.	0.	0.	0.58725319E+09	0.30308251E+03
n_{22}	0.	0.	0.	0.	0.	-0.12553439E-02	0.	0.
n_{23}	0.	0.	0.	0.	0.	-0.76888021E+03	0.	0.
n_{24}	0.	0.	0.	0.	0.	-0.84938358E+03	0.	0.
SATURATION LOCUS								
j_1	-0.32097996E+02	-0.66869126E+01	-0.51504418E+01	0.13814448E+02	-0.95913112E+02	0.67422985E+01	0.13172848E+02	-0.21700826E+01
j_2	0.29976933E+03	-0.20086668E+03	-0.25626822E+03	-0.57396331E+03	0.26738653E+04	-0.11786837E+03	-0.52482838E+03	-0.32255748E+01
j_3	0.70773219E+00	0.37077481E+00	0.26280757E+00	-0.18072036E+00	0.11405373E+01	-0.19946843E+00	-0.18207888E+00	0.23561801E+01
j_4	-0.72349122E-02	-0.62602129E-02	-0.36222681E-02	0.18350292E-02	-0.67026553E-02	0.69680979E-02	0.20385068E-02	-0.95999492E+00
j_5	0.40851153E-04	0.56187159E-04	0.26516635E-04	-0.10957549E-04	0.21745017E-04	-0.14623832E-03	-0.13699320E-04	0.22307327E+00
j_6	-0.12130439E-06	-0.25984366E-06	-0.10004384E-06	0.36123787E-07	-0.37153665E-07	0.17229114E-05	0.51448459E-07	-0.26190467E-01
j_7	0.14448930E-09	0.49025967E-09	0.15423155E-09	-0.50097228E-10	0.26225608E-10	-0.83773053E-08	-0.81676932E-10	0.12190675E-02
SPECIFIC HEAT AT "ZERO" PRESSURE								
m_1	0.79698625E+01	0.29090035E+02	0.29145189E+02	0.25000000E+01	0.51520000E+01	0.10298600E+01	0.10392602E+01	0.51930624E+01
m_2	0.39225023E-02	0.89930170E-03	-0.56919860E-03	0.	0.15224000E-01	0.	-0.50333220E-05	0.
m_3	-0.56781803E-04	-0.92394038E-05	0.68032634E-05	0.	-0.96810061E-05	0.	0.26032523E-07	0.
m_4	0.23442607E-06	0.26008592E-07	-0.48456604E-07	0.	0.23130000E-08	0.	0.	0.
m_5	-0.22395007E-09	-0.14102926E-10	0.13822647E-09	0.	0.	0.	0.	0.
DERIVED PROPERTY CONSTANTS								
T_o	0.11167000E+03	0.77364000E+02	0.90000000E+02	0.87280000E+02	0.19471000E+03	0.27090000E+02	0.68140000E+02	0.42144000E+01
S_o	0.38551735E+01	0.23351167E+01	0.47242694E+01	0.27571770E+01	0.40851019E+01	0.24540781E+01	0.47928763E+01	0.25169600E+01
H_o	0.80320700E+03	0.23118858E+03	0.35642000E+03	0.23793200E+03	0.72665417E+03	0.92348240E+02	0.35387000E+03	0.30033000E+02
CPOCOR	0.26081493E+00	0.35693888E-01	0.31251170E-01	0.20815200E+00	0.95067000E-01	0.10000000E+01	0.10000000E+01	0.10000000E+01
CRITICAL CONSTANTS AND PROGRAM LIMITS								
P_{min}	0.11670000E-01	0.10132000E-01	0.10132500E-01	0.10132500E-01	0.10132000E-01	0.10132500E-01	0.10132500E-01	0.10132000E-01
P_c	0.46270000E+01	0.34170000E+01	0.50830000E+01	0.48650000E+01	0.73835000E+01	0.25537000E+01	0.34986000E+01	0.22746440E+00
P_{max}	0.50670000E+02	0.50670000E+02	0.34000000E+02	0.50660000E+02	0.50669000E+02	0.20290000E+02	0.20270000E+02	0.10132500E+02
T_t	0.90660000E+02	0.64030000E+02	0.54350700E+02	0.83780000E+02	0.21655000E+03	0.24540000E+02	0.68140000E+02	0.30000000E+01
T_c	0.19077000E+03	0.12630000E+03	0.15478000E+03	0.15070000E+03	0.30421000E+03	0.44400000E+02	0.13291000E+03	0.52000000E+01
T_{max}	0.60000000E+03	0.10000000E+04	0.50000000E+03	0.10000000E+04	0.10000000E+04	0.60000000E+03	0.60000000E+03	0.60000000E+03
ρ_c	0.16200000E+00	0.31050000E+00	0.43250000E+00	0.53100000E+00	0.46400000E+00	0.48300000E+00	0.29970000E+00	0.69300000E-01
ρ_t	0.57000000E+00	0.11210000E+01	0.13100000E+01	0.14150000E+01	0.11700000E+01	0.83600000E+00	0.12470000E+01	0.21000000E+00

TABLE III. - A SUMMARY OF PVT RELATIVE ERRORS; FROM FIGURES 1 - 12

(The figure number is in parentheses adjacent to the value of the error.)

Fluid	Investigator	Ref.	Estimated % relative error = 100 (calculated - experimental)/experimental			Range of data			How acquired
			Pressure	Temperature	Density	Pressure, atm	Temperature, ^{o}K	Density or volume	
Methane	Jansoone et al.	58	±0.2 (8)	$^{+0.03}_{-.01}$ (9)	±10 (7)	44.738-49.995	188.946-193.601	68.5926 to 132.4392 cc/gm-mole	Incrementing volume
	Vennix (4 points with errors >10%)	59	±.15 (5)	±.6 (5)	±1.5 (4)	214.03 psia 9935.55 psia	150.03-273.38	0.04088 to .36 gm/cc	
	Vennix*	59	±.03 (2)	±.5 (3)	±.2 (1)	"	"	"	
Oxygen	Weber	31	±2 with a few points at much larger values, see fig. (11)	±0.15 (12)	±0.4 with a max. deviation of ±2 (10)	0.438-357.53	54.5-300.	6.44×10^{-5} to 4.11341×10^{-2} gm-mole/cc	Incrementing temperature
Carbon-dioxide	Michaels et al. Saturated values have been removed.	47	±0.5 with a few points to 5%	±0.1	±3.	36.318-98.497	276.003-313.237	0.10336 to .91507 gm/cc	Various isotherms
Nitrogen	Strobridge	23	-10. to +2.** Much higher values at high densities, see	-4. to +0.5**	-1.3 to +0.8**				
	Coleman-Stewart	60	Very large differences*** at high densities	With higher differences*** at lower temp.	-1.8 to +1.2***				
Helium	McCarty	30	----------	+2 -1 with greater error close to critical point	+2 -1 with up to 20% in critical region	"Data" from the program of McCarty (30).			
Argon	Van Itterbeck et al.	61	±10 with some higher scatter	±0.4	-0.3 to +0.4	10 to 288 atm	90.15 to 148.25	0.795 to 1.439 gm/cc	Various isotherms

*A comparison of the data of Vennix to Vennix's equation of state.

**The Strobridge equation has been overextended to the range up to 1000 K and 100 MN/m^2.

***Equation should not be used below 77 K.

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TABLE IV. - OPERATIONS SHEET FOR SUBROUTINE GASP

```
COMMON/PROPTY/KU, DL, DV, HL, HV, S, SL, SV, CV, CVL, CVV, CP, CPL, CPV, GAMMA, GAMMAL, GAMMAV, C,
CL, CVP, MU, MUL, MUV, K, KL, KV, SIGMA, EXCL, EXCV, EXCESK
REAL MU, MUL, MUV, K, KL, KV
CALL SETUP(NAMGAS)
```

Name the fluid: HE for Helium, CH4 for methane, NE for Neon, N2 for Nitrogen, CO for Carbon Monoxide, O2 for Oxygen, AR for Argon, CO2 for Carbon Dioxide.

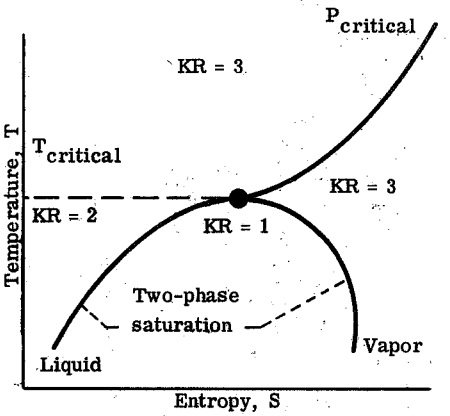
```
CALL GASP(KS, KP, T, P, D, H, KR)
```

- KR — Region
  - KR=0 Unknown, check KR returned
  - KR=1 Saturation
  - KR=2 Liquid
  - KR=3 Gas and or fluid
- H — Enthalpy, J/g
- D — Density, g/cm^3
- P — Pressure, MN/m^2
- T — Temperature, K
- KP — Thermodynamic and Transport properties*

KP=0		Only P, ρ, T returned
KP=1	H	Enthalpy, J/g, (H), (HL), (HV)
KP=2	S	Entropy, J/(g)(K), (S), (SL), (SV)
KP=4	Cv	Specific heat at constant volume, J/(g)(K), (CV), (CVL), (CVV)
	Cp	Specific heat at constant pressure, J/(g)(K), (CP), (CPL), (CPV)
	γ	Ratio of specific heats, Cp/Cv, (GAMMA), (GAMMAL), (GAMMAV)
	c	Sonic velocity, cm/sec, (C), (CL), (CVP)
KP=8	μ	Dynamic viscosity, g/(cm)(sec), (MU), (MUL), (MUV)
KP=16	k	Thermal conductivity, W/(cm)(K), (K), (KL), (KV)
KP=32	σ	Surface tension, dyne/cm, (SIGMA)

- KS — Input specification of independent properties

KS=1	$\rho = f(T,P)$; given T, P find ρ
KS=2	$P = f(T,\rho)$; given T, ρ find P
KS=3	$T = f(p,\rho)$; given P, ρ find T
KS=4	$T,\rho = f(P,H)$; given P, H find T, ρ
KS=5	$T,\rho = f(P,S)$; given P, S find T, ρ



Reset KR≠1 each time GASP is called to be assured of nonsaturation calculations. At the beginning of the user's program, set KU=1 for units indicated above. For other units, see Table V.

SAMPLE PROBLEM

```
COMMON/PROPTY/     (as indicated above)
DATA NAMGAS/2HN2/
CALL SETUP(NAMGAS)
KU=1
CALL GASP(2,31,80,P,1.254,H,KR)
```

The program has been asked to find for nitrogen the pressure P, corresponding to a density of 1.254 g/cm^3 and a temperature of 80 K. Furthermore, the program will return values for H, S, Cv, Cp, γ, C, μ, and k. The values of H and P are returned through the call vector and the remaining values are returned through the COMMON statement.

*For example: KP=1+2=3 will return enthalpy and entropy; KP=1+8+16=25 will return enthalpy, viscosity, and thermal conductivity; KP=1+2+4+8+16=31 returns everything except σ; KP=2 will return entropy.

TABLE V. - UNITS SPECIFICATION KU

Physical quantity	KU=1	KU=2	KU=3
Temperature	K	K	R
Density	gm/cc	gm/cc	lb m/ft^3
Pressure	MN/m^2	atmospheres	psia
Enthalpy	joule/gm	joule/gm	Btu/lb m
Entropy, specific heat	joule/gm-K	joule/gm-K	Btu/lb m-R
Sonic velocity	cm/sec	cm/sec	ft/sec
Dynamic viscosity	gm/cm-sec	gm/cm-sec	lb m/ft-sec
Thermal conductivity	joule/cm-sec-K	joule/cm-sec-K	Btu/ft-sec-R
Surface tension	dyne/cm	dyne/cm	lb_f/ft

KU=4,5 permit the user to work in other units; however, the proper conversions must be entered into BLOCK DATA.

TABLE VI. - PROGRAM ASSEMBLY

1. Set up the return of thermodynamic and transport properties

```
COMMON PRPTY/KU,DL,DV,HL,HV,S,SL,SV,CV,CVL,CVV,CP,CPL,CPV,GAMMA,
     GAMMAL,GAMMAV,C,CL,CVP,MU,MUL,MUV,K,KL,KV,SIGMA,EXCL,EXCV,EXCESK,
     REAL MU,MUL,MUV,K,KL,KV
```

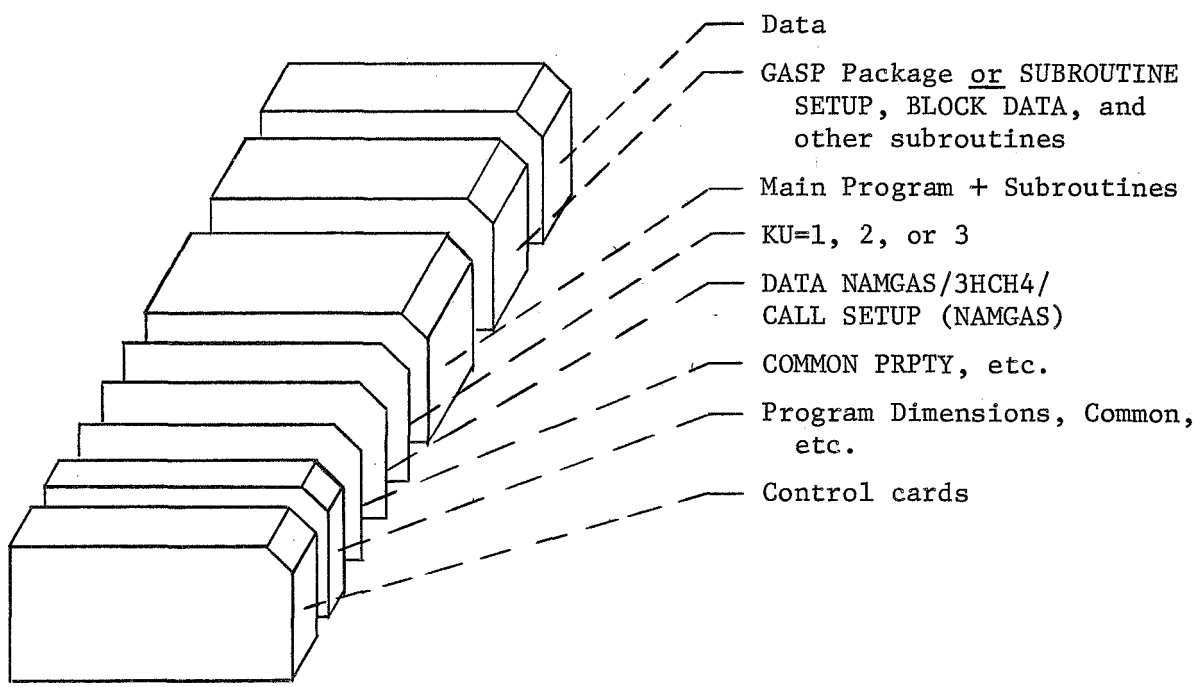
2. Specify the name of the fluid for which properties are required; e.g., DATA NAMGAS/3HCH4/.

3. Call SETUP (NAMGAS). This overlays the proper coefficients. See table II.

4. Establish the units you are working in KU= (specify 1, 2, or 3). See table VI.

5. Add your program here.

6. Add GASP package or SUBROUTINE SETUP (NAMGAS), BLOCK DATA, and other required subroutines.



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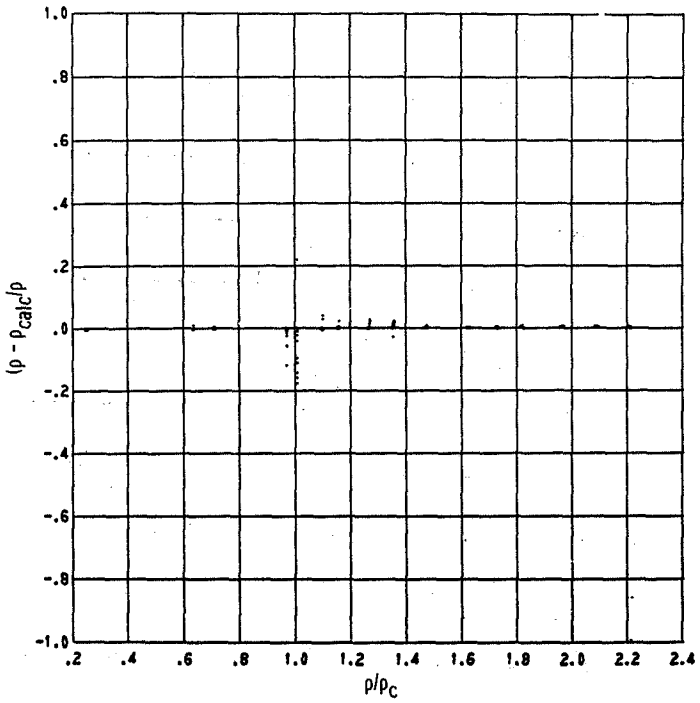


Figure 1. - Relative error in density for the methane data of Vennix, reference 57, as a function of reduced density; calculated values from Vennix's equation of state, reference 57.

CS-60065

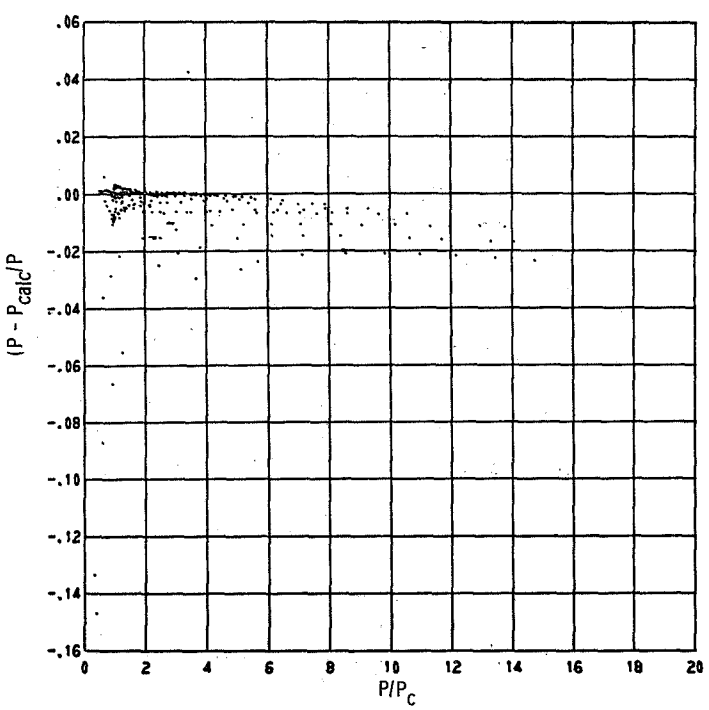


Figure 2. - Relative error in pressure for the methane data of Vennix, reference 57, as a function of reduced pressure; calculated values from Vennix's equation of state, reference 57.

CS-60066

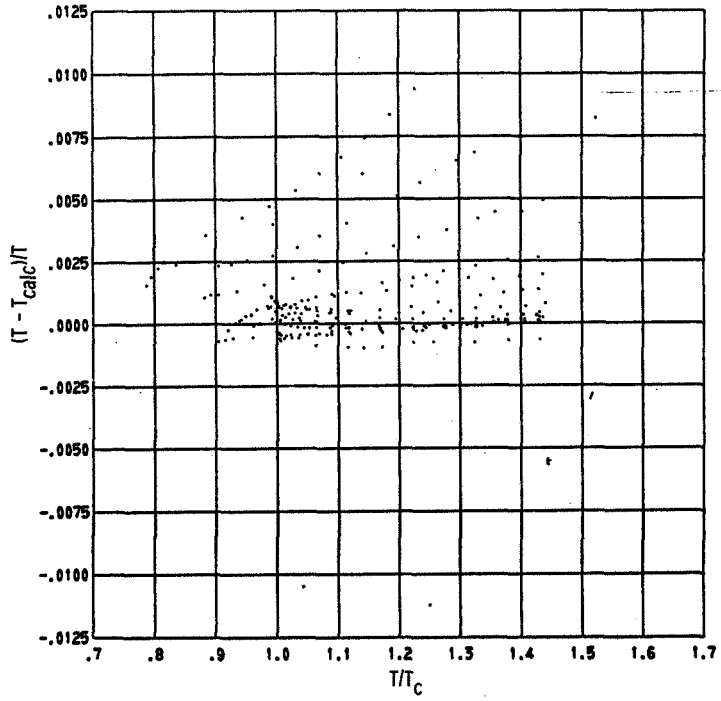


Figure 3. - Relative error in temperature for the methane data of Vennix, reference 57, as a function of reduced temperature; calculated values from Vennix's equation of state, reference 57.

CS-60067

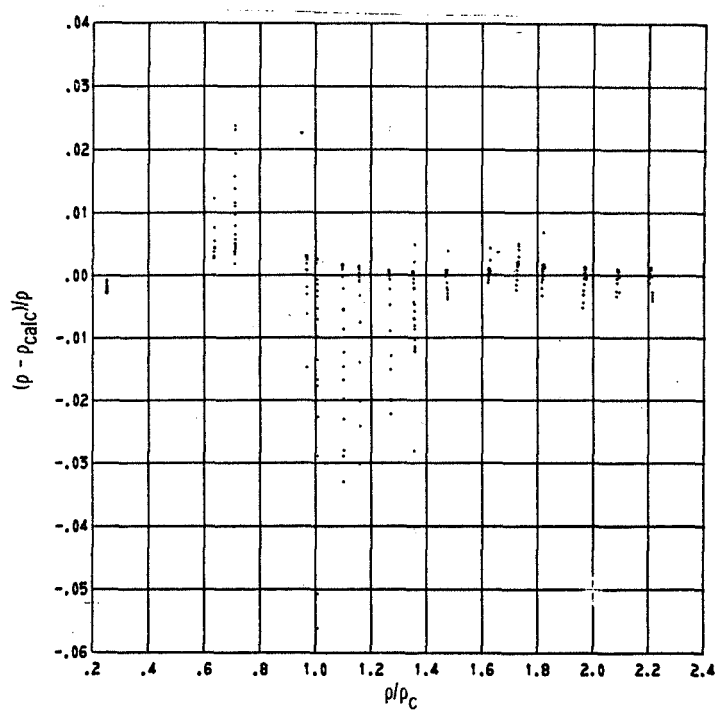


Figure 4. - Relative error in density for the methane data of Vennix, reference 57, as a function of reduced density; calculated values from Bender's equation of state, reference 22.

CS-60068

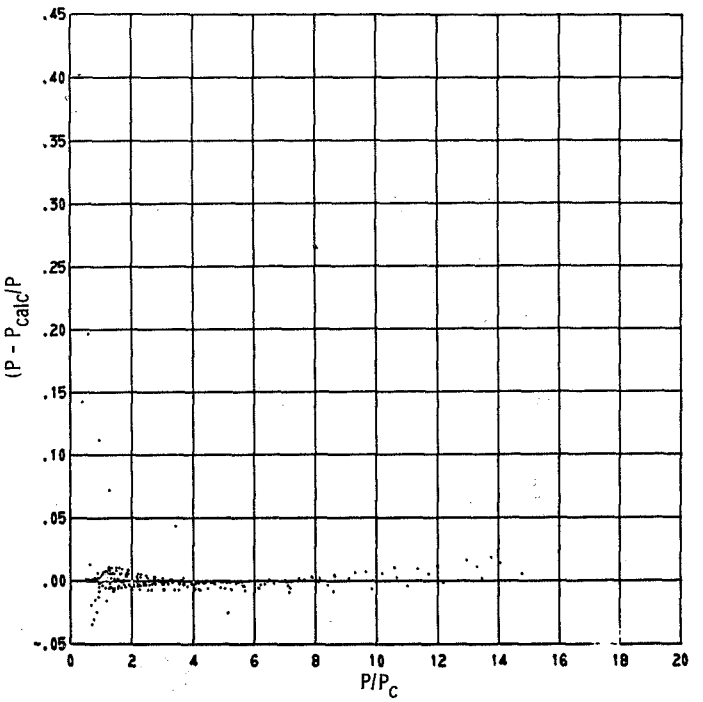


Figure 5. - Relative error in pressure for the methane data of Vennix, reference 57, as a function of reduced pressure; calculated values from Bender's equation of state, reference 22.

CS-60069

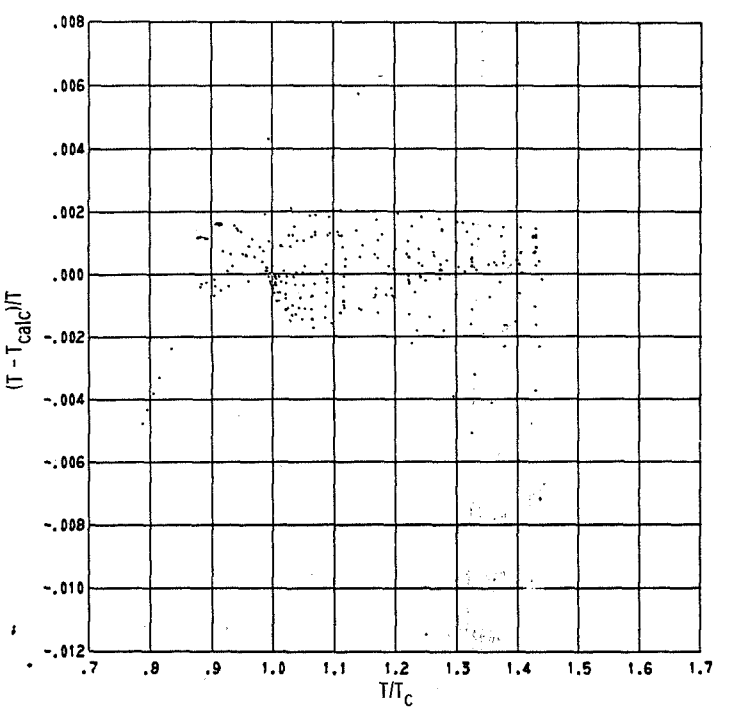


Figure 6. - Relative error in temperature for the methane data of Vennix, reference 57, as a function of reduced temperature; calculated values from Bender's equation of state, reference 57.

CS-60070

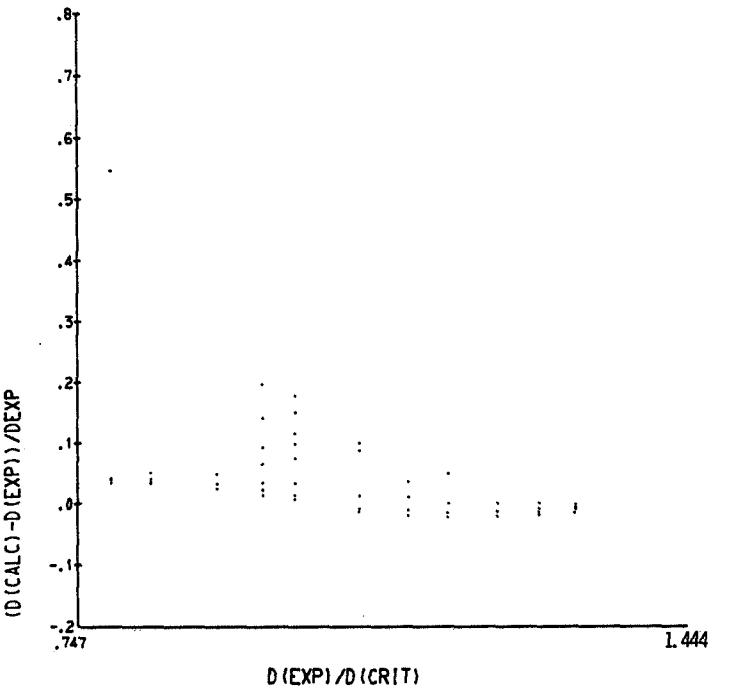


Figure 7. - Relative error in density for the methane data of Jansooue et. al, reference 56 as a function of reduced density; calculated values from Bender's equation of state, reference 22. CS-60071

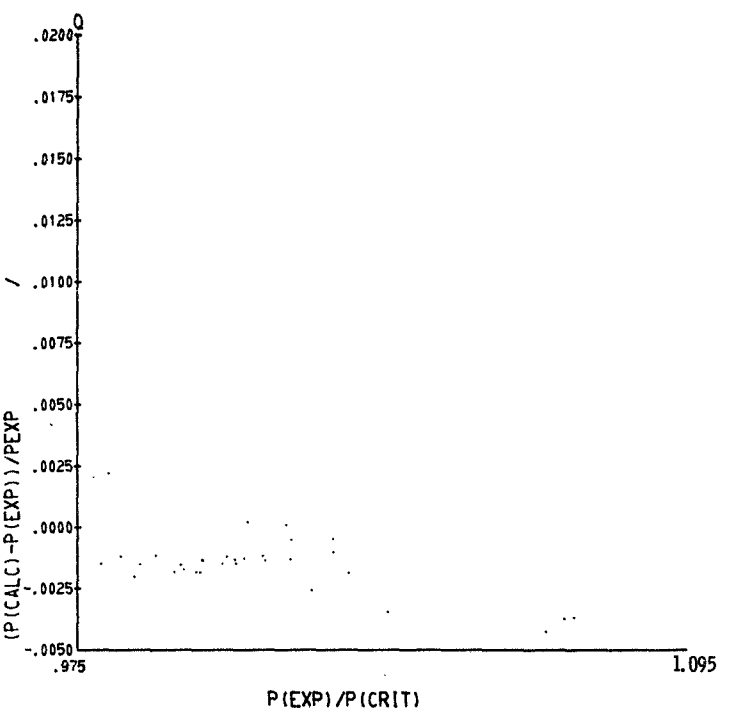


Figure 8. - Relative error in pressure for the methane data of Jansooue et. al, reference 56, as a function of reduced pressure; calculated values from Bender's equation of state, reference 22. CS-60072

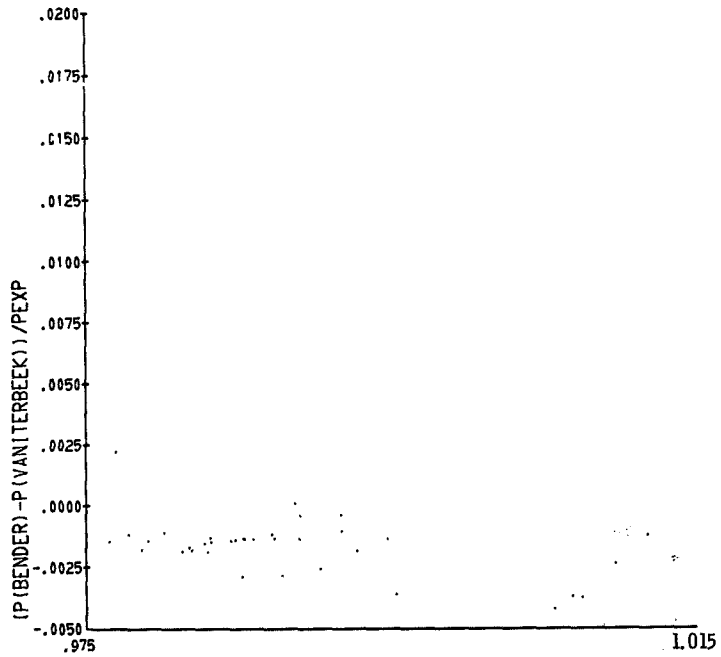


Figure 8. - Concluded. CS-60073

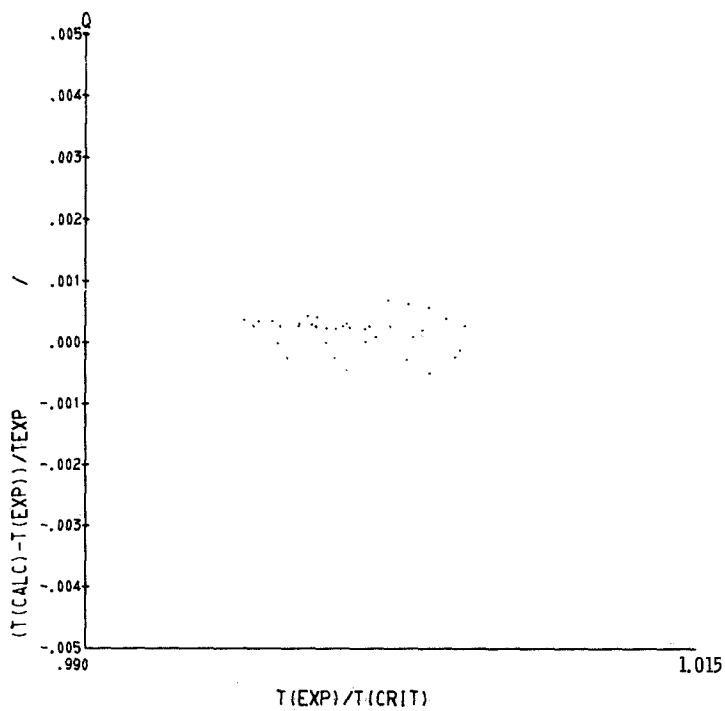


Figure 9. - Relative error in temperature for the methane data of Jansoone et. al, reference 56, as a function of reduced temperature; calculated values from Bender's equation of state, reference 22. CS-60074

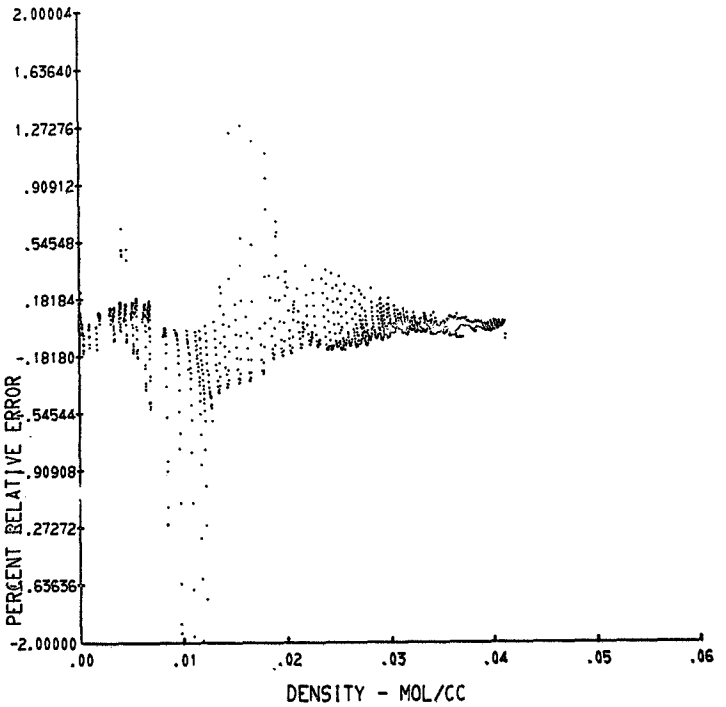


Figure 10. - Relative error in density for the oxygen data of Weber, reference 31, as a function of reduced density; calculated values from Bender's equation of state, reference 22. CS-60075

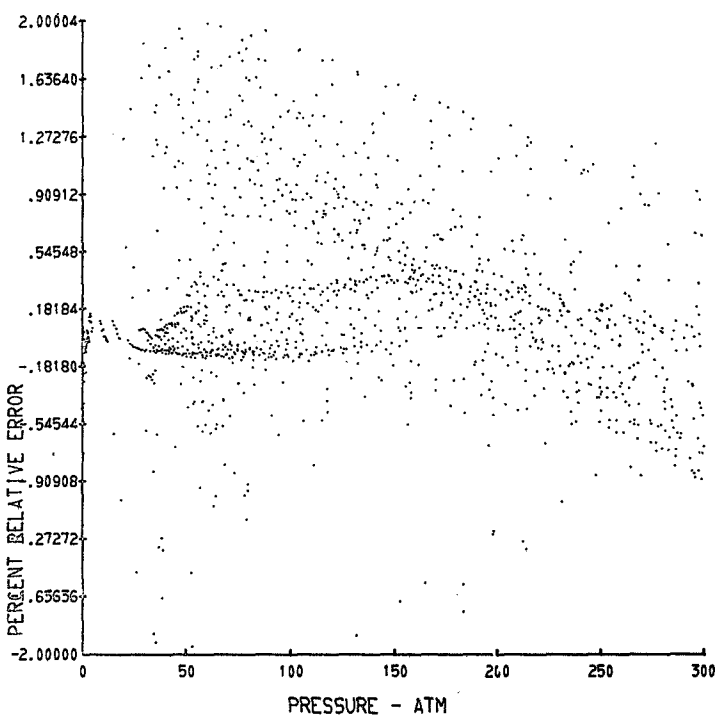


Figure 11. - Relative error in pressure for the oxygen data of Weber, reference 31, as a function of reduced pressure; calculated values from Bender's equation of state, reference 22. CS-60076

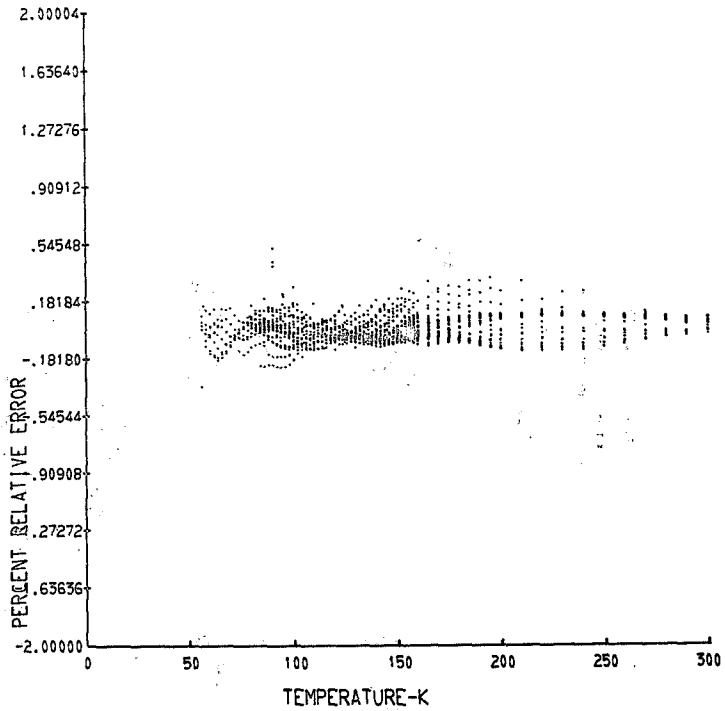


Figure 12. - Relative error in temperature for the oxygen data of Weber, reference 31, as a function of reduced temperature; calculated values from Bender's equation of state, reference 22. CS-60077

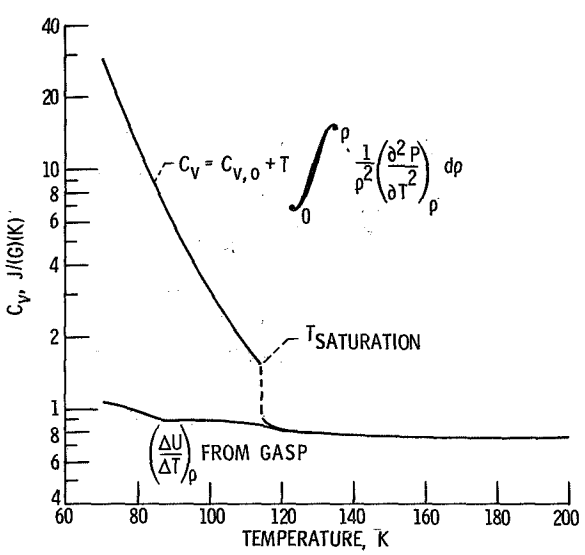
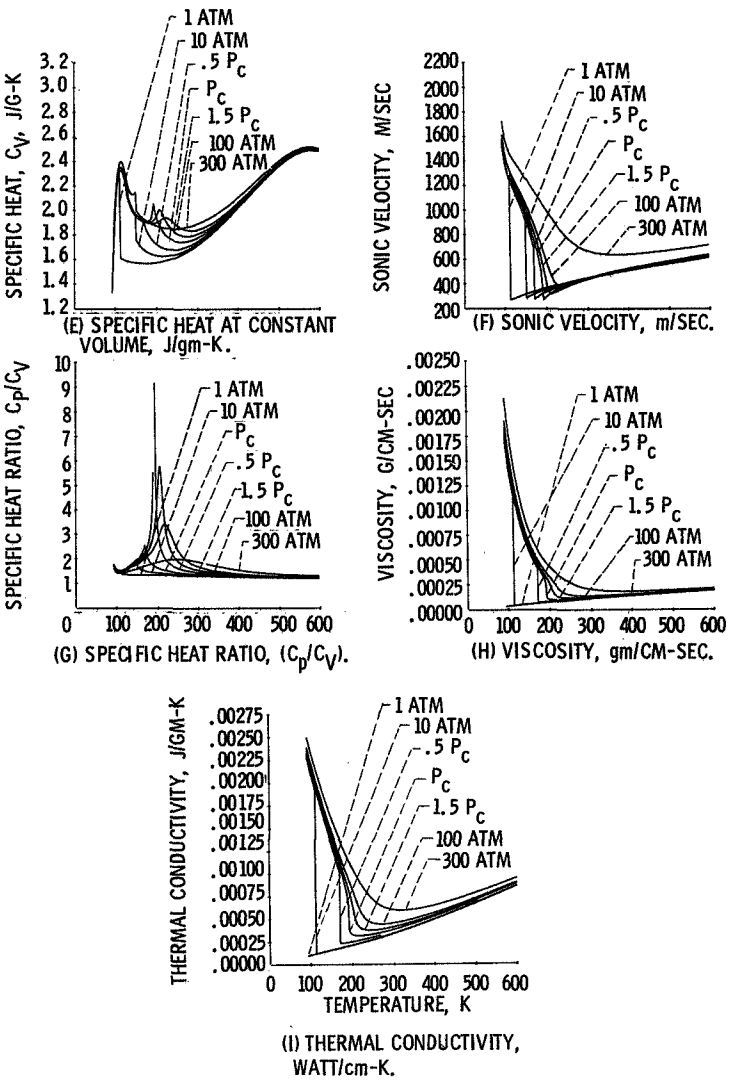


Figure 13. - Behavior of the specific heat at constant volume, Cv, calculated using $\partial^2 P/\partial T^2$ relative to C_V computed from NTWO using $(\Delta U/\Delta T)_\rho$. Pressure = 15 atm.

CS-60078



CS-60062

Figure 14. - Concluded.

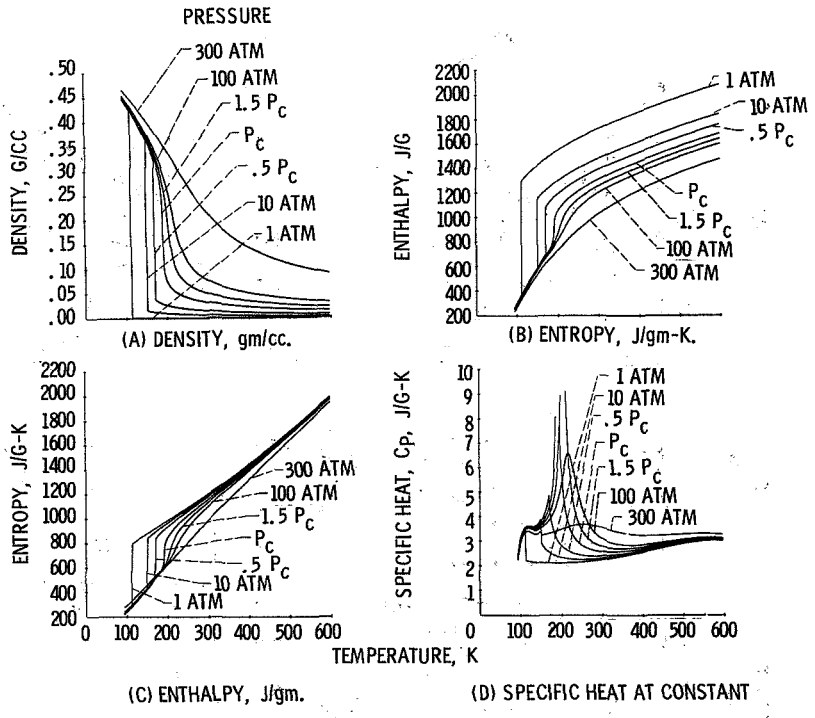


Figure 14. - Thermodynamic and transport properties for fluid methane. CS-60059

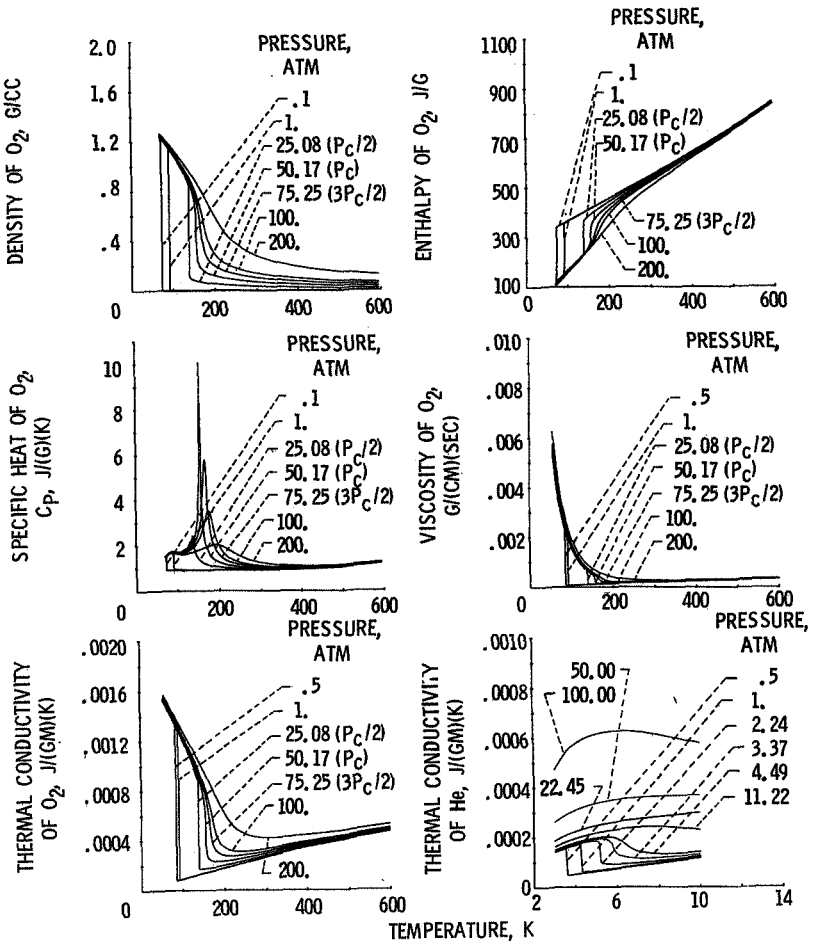


Figure 15. - Selected output from GASP for various isobars of fluids oxygen and helium (0.101 325 * ATM. = MN/M^2).

CS-60061

I NUMERICAL
II NUMERICAL FOR Co, Ne, He
III ANALYTICAL
IV FOR $P < P_c$

$T_c \pm .5$ Co, Ne, He
$T_c \pm .1$ Bender fluids

NEAR CRITICAL REGION OF UNCERTAIN RESULTS IN DERIVED PROPERTIES AND POSSIBLY ρ

NOTE: AT VERY HIGH PRESSURE EXTENSIONS >500 ATM-PROPERTIES AT T_c HAVE BEEN NOTICED.

ρ/ρ_c = 2.5 CH_4
2.2 N_2
2.4 ALL OTHERS

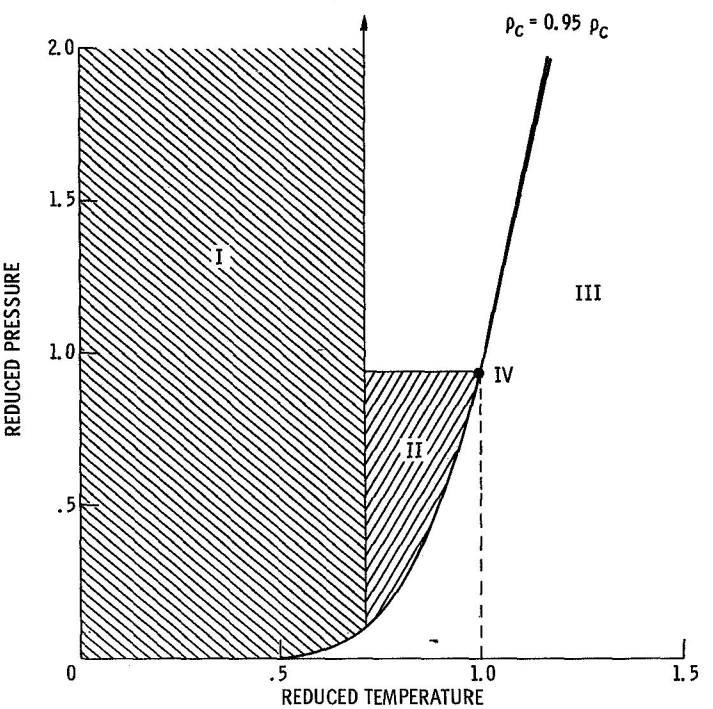


Figure 16. - Analytic and numeric computation regions for specific heat C_V.

CS-60060